International Conference on Secondary Ion Mass Spectrometry

Abstract Book

25-30 October 2026 | Guangzhou, China

https://sims25.scimeeting.cn

1. Welcome Message

Dear SIMS 25 Attendees,

On behalf of the Organizing Committee, it is our great pleasure to welcome you to the 25th International Conference on Secondary Ion Mass Spectrometry (SIMS 25) in Guangzhou, China.

Convening in China for the first time, SIMS 25 celebrates global connection, intellectual discourse, and frontier exploration. As a historic gateway of the Maritime Silk Road and a vibrant center of the Guangdong–Hong Kong–Macao Greater Bay Area, Guangzhou carries forward a legacy of openness and cultural exchange.

In this spirit, the SIMS community brings together advances in fundamental research, technological breakthroughs, and emerging applications, including:

- Fundamentals & Instrumentation
- AI, Machine Learning and Data Analysis
- Earth and Environmental Sciences
- Materials Science
- Life Sciences
- Industrial Applications
- Correlated Analysis
- Special Session – Atom Probe Tomography (APT)

We are honored to welcome our distinguished plenary and invited speakers, alongside experts leading pre-conference tutorials. We also extend our deepest appreciation to all speakers, session chairs, committee members, sponsors, and participants whose contributions and support bring this landmark event to life.

We look forward to stimulating discussions, new perspectives, and lasting collaborations, and wish you a productive and memorable conference!

Sincerely



Chair of SIMS 25

2. Conference Committee

2.1 Conference Chair

Lu-Tao Weng (The Hong Kong University of Science and Technology (Guangzhou)) Guangzhou, China)

2.2 Conference Co-Chairs

Xian-Hua Li (Institute of Geology and Geophysics, Beijing, China)

Yuan Wu (University of Science and Technology Beijing, Beijing, China)

Lixia Zhao (Tiangong University, Tianjin, China)

2.3 International Scientific Committee

Morgan Alexander (University of Nottingham, UK)

Satoka Aoyagi (Seikei University, Japan)

Jean-Paul Barnes (CEA Leti in Grenoble, France)

Anna Belu (Medtronic, USA)

Caroline Bouvier (University of Maastricht, Netherlands)

Arnaud Delcorte (Université Catholique de Louvain, Belgium)

Andrew Ewing (University of Gothenburg, Sweden)

John Fletcher (University of Gothenburg, Sweden)

Alexis Franquet (IMEC, Belgium)

Lara Gamble (University of Washington, USA)

Greg Gillen (NIST, USA)

Ian Gilmore (NPL, UK)

Ron Heeren (University of Maastricht, Netherlands)

Marco Hopstaken (IBM, USA)

Laurent Houssiau (University of Namur, Belgium)

Trevor Ireland (The University of Queensland, Australia)

Haibo Jiang (The University of Hong Kong)

Manuela Killian (Universität Siegen, Germany)

Tae Geol Lee (KRISS, Korea)

Yeonhee Lee (Korea Institute of Science and Technology, Korea)

Antonino Licciardello (University of Catania, Italy)

Haiyang Li (Dalian Institute of Chemical Physics, China)

Xian-Hua Li (Institute of Geology and Geophysics, China)

Nick Lockyer (University of Manchester, UK)

Christine Mahoney (Corning Incorporated, USA)

Jiro Matsuo (Kyoto University, Japan)

Dae Won Moon (DGIST, Korea)

Ewald Niehuis (IONTOF, Germany)

Satoshi Ninomiya (University of Yamanashi, Japan)

Michaeleen Pacholski (Dow Chemicals, USA)

Zbigniew Postawa (Jagiellonian University, Poland)

Peter Sjovall (SP Technical Research Institute of Sweden, Sweden)

Hua Tian (University of Pittsburgh, USA)

Fuyi Wang (Institute of Chemistry, China)

Lu-Tao Weng (HKUST(GZ), China)

Yuan Wu (University of Science and Technology Beijing, China)

Martin Whitehouse (Swedish Museum of Natural History, Sweden)

Tom Wirtz (LIST, Luxembourg)

Hisayoshi Yurimoto (Hokkaido University, Japan)

Zhihua Zhu (Pacific Northwest National Laboratory, USA)

2.4 Local Committee

2.4.1 Advisory Committee

Dunyi Liu (Institute of Geology)

Yong Chien Ling (National Tsinghua University, Hsinchu/Taiwan)

2.4.2 Local Organization Committee

Jian Chen (Sun Yat-Sen University)

Sunan Ding (Nanjing University)

Dong Gui (TSMC, Taiwan)

Rong Hu (Nanjing Technology University)

Younan Hua (Wintech Nano (Suzhou) Co. Ltd)

Haibo Jiang (The University of Hong Kong)

Haiyang Li (Dalian Institute of Chemical Physics)

Hui Li (Shanghai University)

Qiuli Li (Institute of Geology and Geophysics)

Xian-Hua Li (Institute of Geology and Geophysics)

Zhanping Li (Tsinghua University)

Handong Liang (China University of Mining and Technology)

Tao Long (Institute of Geology)

Fu-De Mai (Taipei Medical University)

Gang Sha (Nanjing University of Science and Technology)

Fuyi Wang (Institute of Chemistry)

Lu-Tao Weng (Hong Kong University of Science and Technology (Guangzhou))

Yuan Wu (University of Science and Technology Beijing)

Xiaoping Xia (Guangzhou Institute of Geochemistry)

Wei Yang (Institute of Geology and Geophysics)

Lei Zhang (Institute of Metal Research)

Lixia Zhao (Tiangong University)

2.5 International Committee

Arnaud Delcorte (Université Catholique de Louvain, Belgium)(Chair)

Christine Mahoney (Corning, USA)(Secretary)

Satoka Aoyagi (Seikei University, Japan)

Jean-Paul Barnes (CEA Leti in Grenoble, France)

David Carr (3M, USA)

Michael Eller (California State University, USA)

Lara Gamble (University of Washington, USA)

Tae Eun Hong (Korea Basic Science Institute, Korea)

Haibo Jiang (The University of Hong Kong, China)

Manuela Killian (Universität Siegen, Germany)

Nick Lockyer (University of Manchester, UK)

Lu-Tao Weng (HKUST(GZ), China)

3. Conference information

3.1 Presentation Durations

Plenary Talk: 60 min (including Q&A)

Invited Talk: 40 min (including Q&A)

Oral Presentation: 20 min total (15 min presentation + 3 min discussion + 2 min Q&A)

Note: Exact timing is subject to the Session Chair's discretion.

3.2 Friendly Reminders

- In each session, the discussion order will be managed by the session chair.
- Presentation Preparation & Data Security: Speakers must copy their PDF/PPT files to the designated venue computer in advance.
- Conference photography will take place during the sessions. In case of non-consent, please inform the organisers.
- Assurance: All PPT files will be deleted immediately after the session, with no risk of data leakage.

3.3 Punctuality & Seating

Speakers must arrive 15 minutes before the session and take their seats in the front row. If delayed, notify the session chair in advance.

4. General Information

4.1 Registration Desk

Venue: Foyer, Nansha Bay Marina Convention Center

Date and Time:

15:00-19:00 (GMT+8), October 24

08:30-18:00 (GMT+8), October 25 - 27, 29

08:30-13:00 (GMT+8), October 28

08:30-12:00 (GMT+8), October 30

4.2 Welcome Reception

Venue: Grand Ballroom, LN Garden Hotel Nansha Guangzhou

Date and Time: 17:30 - 20：30, October 25

4.3 Lunch

Venue: Garden All-Day Dining Restaurant (Café Flora), LN Garden Hotel Nansha Guangzhou

Date & Time:

12:30 - 14:00 (GMT+8), October 25

13:00 - 14:00 (GMT+8), October 26

12:00 - 13:00 (GMT+8), October 28

4.4 Poster Reception

Venue: Foyer, Nansha Bay Marina Convention Center

Date & Time: 12:40-15:00, October 27, 29

4.5 Cultural Tour & Banquet & Pearl River Night Cruise

Guangzhou Cultural Tours：13:00 - 19:00, October 28

Meeting Point: Lobby, LN Garden Hotel Nansha

Banquet：19：00 - 20:30, October 28

Venue: Bingsheng Seafood Restaurant

Pearl River Night Cruise: 20:30 - 22:30, October 28

Venue：Dashatou Yuexiu District

4.6. Notes

Assembly Time & Location: Please prepare your belongings in advance and gather at the Lobby of LN Garden Hotel Nansha BEFORE 13:00. The group will depart promptly.

Dress Code & Footwear: Please wear comfortable, casual clothes and suitable walking shoes, as the cultural tour will involve moderate walking.

Weather & Evening Breeze: As the boat cruise takes place outdoors in the evening, it may get chilly and windy on the river. We strongly recommend bringing a light jacket or cardigan.

What to Bring:

A valid ID or passport (required for security check at the cruise terminal) and your conference badge.

Personal essentials (e.g., umbrella/sunshade, power bank, personal medications).

25th International Conference on Secondary Ion Mass Spectrometry

OVERVIEW PROGRAM

25–30 October 2026
Guangzhou, China

Sunday 25 Oct. — Tianhai Room 2

Tutorial 1
09:00-10:00
A. Delcorte
Université catholique de Louvain

Coffee break

Tutorial 2
10:30-11:30
P. Michałowski
Lukasiewicz Research Network - Institute of Microelectronics and Photonics

Tutorial 3
11:30-12:30
K. Moore
University of Manchester

Lunch

Tutorial 4
14:00-15:00
S. Aoyagi
Seikei University

Coffee break

Tutorial 5
15:30-16:30
R. Hu
Nanjing Tech University

Welcome Reception
17:30-20:30

Monday 26 Oct. — Yunhai

Opening Ceremony
09:00-09:30
Welcome & opening of SIMS25

PL1 - Alfred Benninghoven Award
09:30-10:30
J. Matsuo
QSEC, Kyoto University

Coffee break

Tianhai Room 1	Tianhai Room 2	Tianhai Room 3
COR 1-1 (H)	IND 1-2 (G)	MAT 1-3 (E)
11:00 Y. Ying (I)	11:00 C. Mahoney (I)	11:00 D. Wu
		11:20 K. Khosravani
11:40 R. Webb	11:40 F. Scholz	11:40 P. Michałowski
12:00 M. Brajković	12:00 L. Tan	12:00 Y. Zhao
12:20 R. Schusterbauer		

Lunch
12:40-14:00

DAT 2-1 (C)	COR 2-2 (H)	LIF 2-3 (F)
14:00 J. Fletcher (I)	14:00 J. P. Barnes (I)	14:00 Y. Liang
		14:20 C. Newell
14:40 A. Henderson	14:40 P. Sjövall	14:40 G. Di Stadio
15:00 Z. Tang	15:00 K. Moore	15:00 M. Alexander
15:20 M. Eller	15:20 Y. Su	15:20 J. L. Lu (Jennifer)

Coffee break

GEO 3-1 (D)	LIF 3-2 (F)	FUN 3-3 (A)
16:00 Y. Guan (I)	16:00 L. Thornton	16:00 Z. Postawa (I)
	16:20 M. Lakhdar	
16:40 X. Li	16:40 K. Zwolenik	16:40 P. Gherardi
17:00 J. Wang	17:00 Y. Jin	17:00 Y. Mizutani
17:20 D. M. Galindo	17:20 N. Gotzmann	17:20 J. Ekar

Tuesday 27 Oct. — Yunhai

PL2 - Plenary Lecture
09:00-10:00
A. Ewing
University of Gothenburg

Diamond Sponsor Talks
10:00-10:15 IONTOF
10:15-10:30 RAITH

Coffee break

Tianhai Room 1	Tianhai Room 2	Tianhai Room 3
INS 4-1 (B)	LIF 4-2 (F)	APT 4-3 (I)
11:00 J.-N. Audinot (I)	11:00 H. Jiang (I)	11:00 G. Schmitz (I)
11:40 A. Auditore	11:40 N. Valle	11:40 Y. Feng
12:00 D. Rading	12:00 A. Smits	12:00 F. Zhang
	12:20 A. Cichy	

Poster Session 12:40-15:00 | Venue: Foyer
Exhibition & refreshments
Lunch 12:40-15:00

MAT 5-1 (E)	FUN 5-2 (A)	INS 5-3 (B)
15:00 J. Zhang	15:00 M. Lagator (I)	15:00 A. Ost
15:20 L. Zhang		15:20 P. Peres
15:40 V. Graziani	15:40 A. Delcorte	15:40 G. Azimi
16:00 Y. Hua	16:00 S. Sheraz	16:00 I. Gilmore (I)
16:20 M. Rohnke	16:20 K. Moritani	
16:40 Y. Lee	16:40 S. Ninomiya	

Sponsor Workshop Raith 17:00-18:00
Sponsor Workshop CAMECA 17:00-18:00
Sponsor Workshop PHI 17:00-18:00

Wednesday 28 Oct. — Yunhai

PL3 - Plenary Lecture
09:00-10:00
Q. Li
Institute of Geology and Geophysics
Chinese Academy of Sciences

Diamond Sponsor Talks
10:00-10:15 CAMECA
10:15-10:30 PHI

Coffee break

SIMS Meeting Presentation
11:00 Presentation of SIMS 26 (2028)
11:10 Presentation of SIMS Europe (2027)
11:20 Presentation of SIMS China (2027)
11:30 Conference Photo

Lunch

Cultural Tour and Banquet
Starting from 13:00

Thursday 29 Oct.

Tianhai Room 1	Tianhai Room 2	Tianhai Room 3
INS 6-1 (B)	LIF 6-2 (F)	APT 6-3 (I)
09:00 H. Li (I)	09:00 J. Kovač	09:00 Y. Wu
	09:20 N. Phan	
09:40 G. Zhu	09:40 X. Li	09:40 S. W. Hung
10:00 S. Miwa	10:00 A. Srivastava	10:00 F. Vogel

Coffee break
10:20-11:00

Tianhai Room 1	Tianhai Room 2	Tianhai Room 3
IND 7-1 (G)	MAT 7-2 (E)	LIF 7-3 (F)
11:00 D. Gui (I)	11:00 Y. Zhang (I)	11:00 H. Tian (I)
11:40 Z. Guan	11:40 T. Weintraut	11:40 I. Dar
12:00 T. Ohashi	12:00 N. Sano	12:00 M. Sun
12:20 H. Liu	12:20 A. Henss	12:20 M. Takeuchi
12:40 J. Viggars	12:40 Z. Daher	12:40 F. Fahrnberger

Poster Session 13:00-15:00 | Venue: Foyer
Exhibition & refreshments
Lunch 13:00-15:00

LIF 8-1 (F)	MAT 8-2 (E)	DAT 8-3 (C)
15:00 T. Lee (I)	15:00 V. Thoréton	15:00 K. Li
	15:20 M. Killian	15:20 S. Aoyagi
15:40 L. Milne	15:40 M. S. Russo	15:40 J. Barrette
16:00 N. Lockyer	16:00 N. Zhou	16:00 M. Hayase
16:20 G. Kanclerz	16:20 M. Dürr	16:20 F. Mai
16:40 M. Consumi	16:40 D. Scurr (I)	16:40 Z. Wang
17:00 C. Dieterle		17:00 J. Liu

Sponsor Workshop IONTOF 17:20-18:20
Sponsor Workshop IONOPTIKA 17:20-18:20

Friday 30 Oct.

Tianhai Room 1	Tianhai Room 2	Tianhai Room 3
GEO 9-1 (D)	MAT 9-2 (E)	COR 10-3 (H)
09:00 H. Yurimoto (I)	09:00 V. B. Olmos	09:00 R. Tilmann (I)
	09:20 X. Zeng	
09:40 O. Yang	09:40 J. Ren	09:40 G. Zhu
10:00 K. Norrman	10:00 G. Munier-Gondiant	10:00 T. Seki
	10:20 H. Y. Nie	10:20 G. Medeiros-Ribeiro

Coffee break
10:40-11:00

Tianhai Room 1	Tianhai Room 2	Tianhai Room 3
GEO 10-1 (D)	MAT 10-2 (E)	
11:00 M. Krmpotić	11:00 L. Tortora	
11:20 N. Sakamoto	11:20 V. Spampinato	
	11:40 L. Houssiau	

Closing & Award Ceremony
12:00-12:30

TOPICS
A Fundamentals | B Instrumentation | C AI, Machine Learning & Data Analysis | D Earth & Environmental Sciences | E Materials Science
F Life Sciences | G Industrial Applications | H Correlated Analysis | I Special Session — Atom Probe Tomography

Remark: Click any session or speaker name to jump directly to the corresponding abstract page.

Interactive program preview

Focused Ion Beams

RAITH

IONMASTER

Magnetic sector SIMS analysis for nm-scale elemental mapping

< 25 nm SIMS imaging resolution

Fastest time to result with full-mass-spectrum acquisition

Automated sample navigation with highest precision

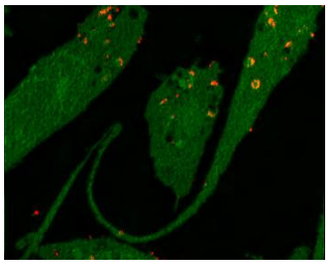


raith.com

RAITH

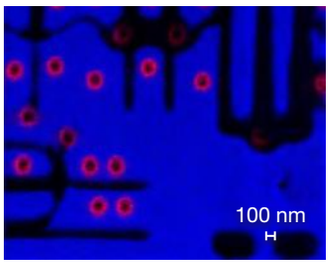
IONMASTER

The right solution to drive innovation



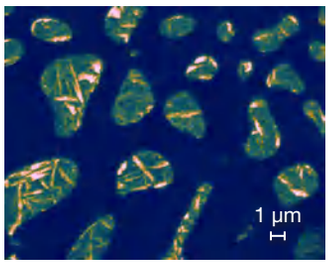
Life Science

Highest sensitivity



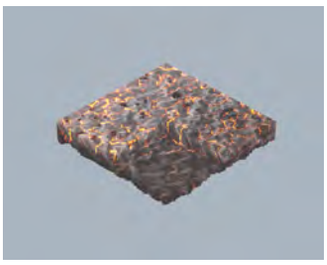
Semi-conductor

Fast results and automation



Materials Science

Sub 25 nm lateral resolution



Green Energy

Exact 3D reconstructions

About us

RAITH is the global market and technology leader in maskless nanofabrication systems and characterization solutions. With our unique combination of high-precision products, integrated solutions, and proprietary technologies, we drive innovation and accompany a wide variety of industries and applications.



> 50	500	> 1,300	10
years of experience	employees worldwide	Instruments installed	offices worldwide with 3 experience centers

Atomic Level Characterization using ULVAC-PHI Surface Analysis Instruments

Comprehensive solution for batteries, semiconductors, organic devices and other applications

Latest Generation of TOF-SIMS

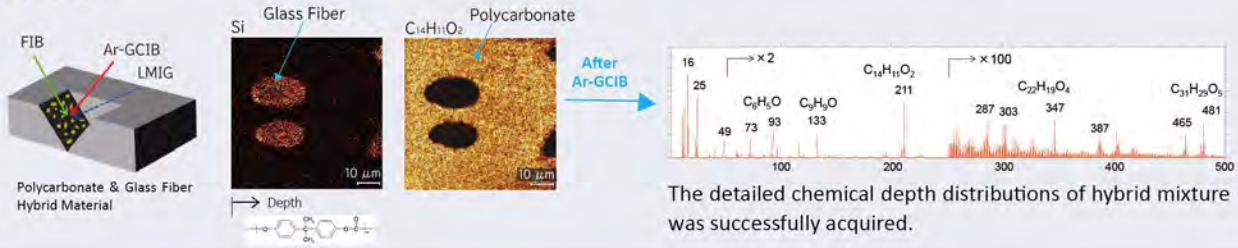
PHI nanoTOF 3^{+}

- High-Precision Analysis with TRIFT Analyzer
- Continuous Unattended Measurement of Insulating Materials
- Unique Ion Beam Technology
- Molecular Structure Analysis Based on Parallel Imaging MS/MS
- A Wide Selections of Options



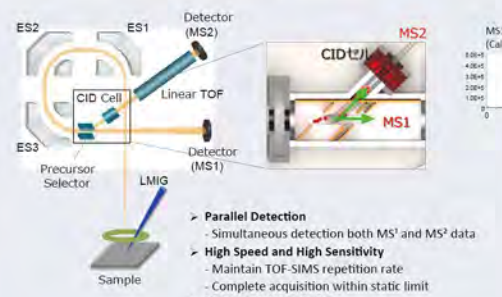
in-situ FIB Cross Sectioning

Cross-section Imaging of Inorganic/Organic Hybrid Materials Using FIB-TOF-SIMS

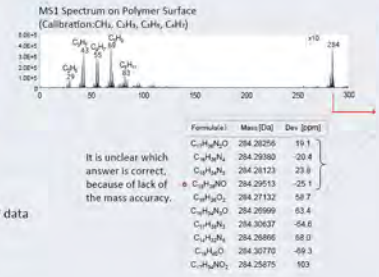


The detailed chemical depth distributions of hybrid mixture was successfully acquired.

TOF-SIMS with Parallel Imaging MS/MS

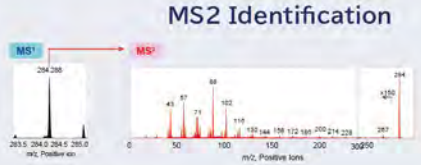


- **Parallel Detection**
  - Simultaneous detection both MS^1 and MS^2 data
- **High Speed and High Sensitivity**
  - Maintain TOF-SIMS repetition rate
  - Complete acquisition within static limit
- **High Spatial Resolution**
  - Bismuth cluster ions are available for MS^2 analysis
- **Mass Selection Window < 1 Da**
  - Easy Interpretation of MS^2 spectra



Formula(-)	Mass [Da]	Dev [ppm]
$C_{17}H_{32}N_2O$	284.26256	19.1
$C_{18}H_{36}N_2$	284.29380	-20.4
$C_{19}H_{40}N_2$	284.28123	23.8
$C_{18}H_{38}NO$	284.29513	-25.1
$C_{19}H_{36}O_2$	284.27132	58.7
$C_{18}H_{36}N_2O$	284.28999	63.4
$C_{17}H_{36}N_3$	284.30637	-54.6
$C_{16}H_{38}N_4$	284.26866	58.0
$C_{18}H_{40}O$	284.30770	-69.3
$C_{17}H_{40}NO_2$	284.25875	103

It is unclear which answer is correct, because of lack of the mass accuracy.



The answer is " $C_{18}H_{38}NO$ " !

ULVAC-PHI, INC.

ULVAC-PHI, Inc.
2500 Hagisono, Chigasaki, Kanagawa, 253-8522, Japan
Phone:81-467-85-4220 Fax:81-467-85-4411

www.ulvac-phi.com

Quadrupole Secondary Ion Mass Spectrometer

Outstanding performance for ultra fast depth profiling

PHI ADEPT 2

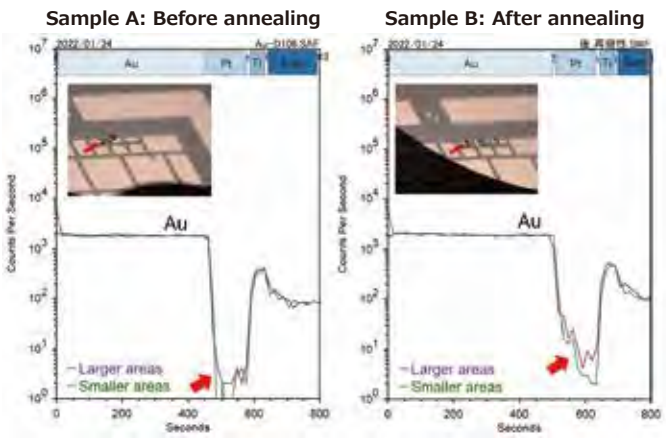
New Product

PHI ADEPT 2 is a next-generation quadrupole SIMS system offering further advancements in analytical performance.
Its newly designed lens column and power supply deliver high-sensitivity elemental analysis, excellent depth resolution, and outstanding system stability.
In addition, SmartSoft-SIMS enables intuitive and seamless operation.

- **Advanced Automated Analysis**
- **High-Speed, High-Sensitivity Depth Profiling**
- **Ultimate Depth Resolution**
- **Ultimate Detection Limits through Ultra-High Vacuum**

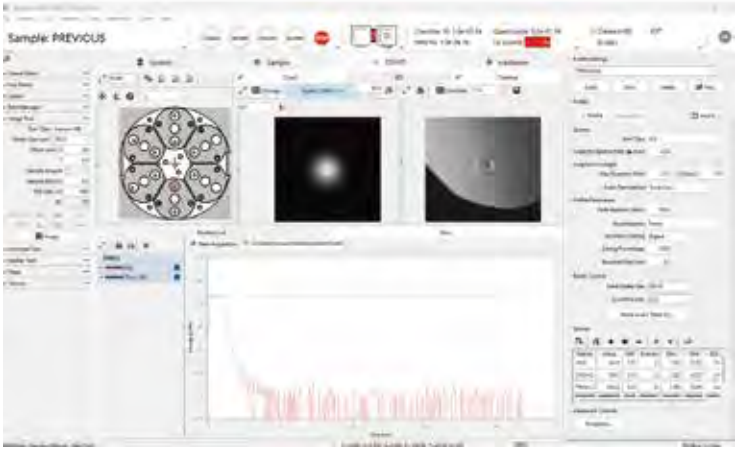


New Column Lens Enables Easy Analysis of Patterned Samples

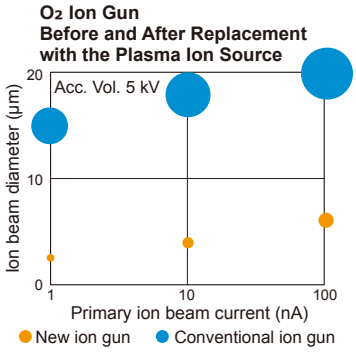


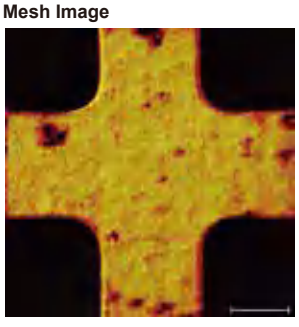


Smart and Intuitive Operation with SmartSoft-SIMS



Optional ICP Ion Source Enables an Even Smaller Oxygen Ion Beam





ULVAC-PHI, INC.



The M6

Advanced Ion Beam Technology for Surface Analysis

Advanced Ion Beam Technology for Surface Analysis

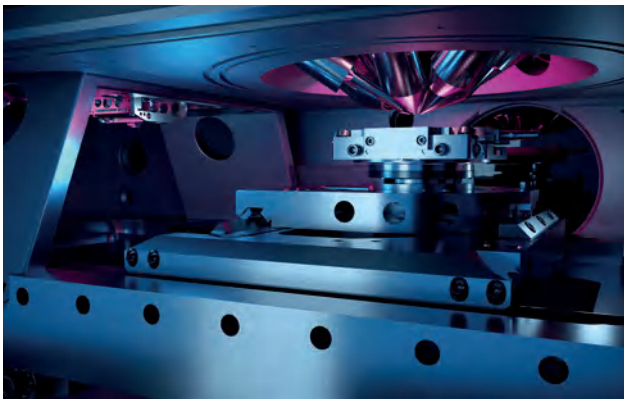
M6



Superior SIMS Performance

The M6 is the latest generation of high-end TOF-SIMS instruments developed by IONTOF. Its design guarantees superior performance in all fields of SIMS applications.

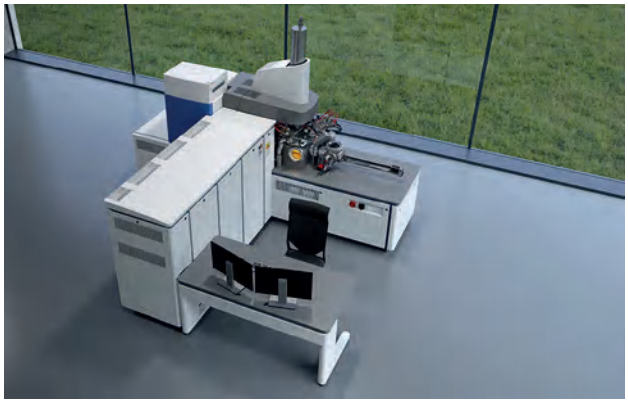
M6 Plus



SIMS and SPM in situ

The M6 Plus is the tool for nano characterisation. Combining high-end performance SIMS and SPM, true in situ 3D chemical imaging becomes possible.

M6 Hybrid SIMS



High-end Mass Spectrometry

With the Orbitrap™ extension for the M6, IONTOF introduces the first commercial SIMS instrument combining highest mass resolution and mass accuracy with high resolution cluster SIMS imaging.

Qtac



Top Atomic Layer Analysis

The Qtac is a high sensitivity low energy ion scattering (LEIS) instrument. It is extremely surface sensitive, providing small spot quantitative elemental characterisation of the top atomic layer.

Heisenbergstraße 15
48149 Münster
Germany

Phone: +49 251 1622-100
Email: sales@iontof.com
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IONTOF

IMS 8f: AUTOMATED DYNAMIC SIMS FOR SEMICONDUCTOR AND ADVANCED MATERIALS CHARACTERIZATION

CAMECA
SCIENCE & METROLOGY SOLUTIONS
AMETEK

A new platform for advanced analytical challenges

Automated operation. Analytical versatility.
Proven magnetic sector SIMS performance.
From light elements and complex interfaces to shallow structures and deep profiles.



AUTOMATED ALIGNMENT

Less tuning. More understanding.

IMS 8f automates primary and secondary column alignment through a streamlined workflow, shortening time to measurement and delivering more consistent operating conditions. The result is better day-to-day reproducibility and more productive use of operator time, allowing greater focus on analytical insight rather than instrument setup.

- Shorter time to measurement
- Better day-to-day reproducibility
- More productive operator time

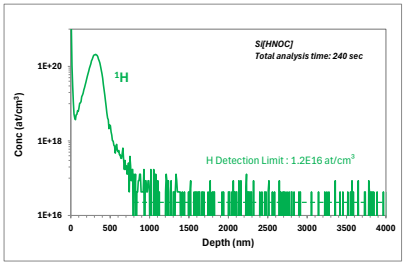
Automated Alignment
Primary and secondary column alignment

Expanded Analytical Foundation
New Cs source, PBMF architecture and improved vacuum design

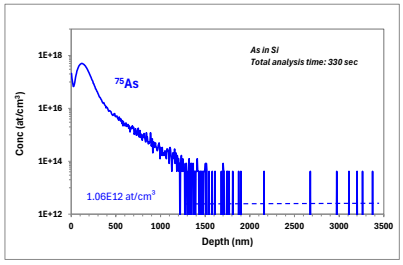
Industrial Platform
New electronics and semiconductor deployment requirements

APPLICATIONS

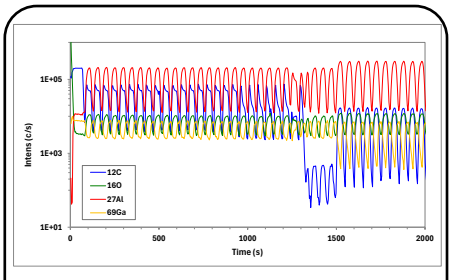
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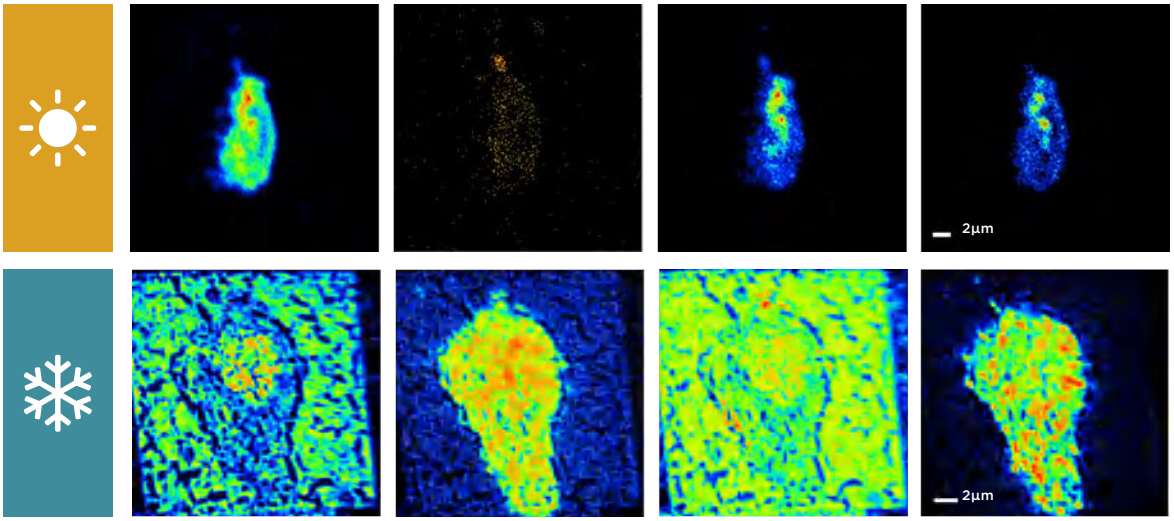
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Silvio Rizzoli
Full Professor, Chair of Neuro & Sensory Physiology Department, University Medical Center Göttingen, Germany



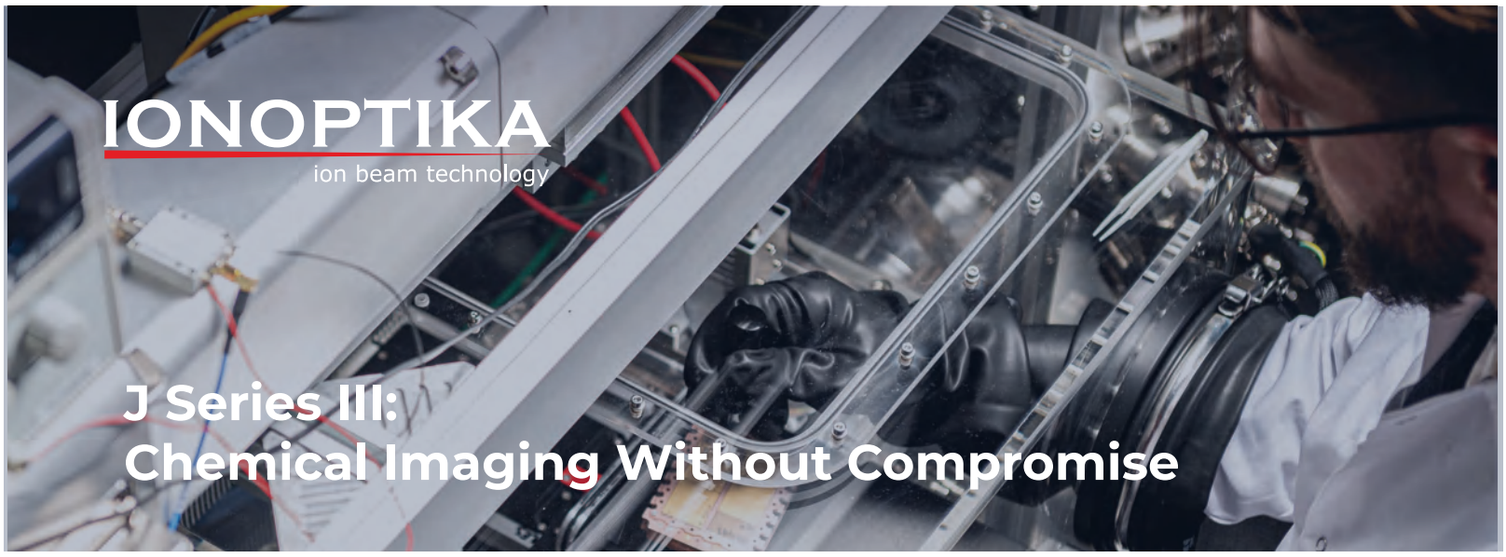
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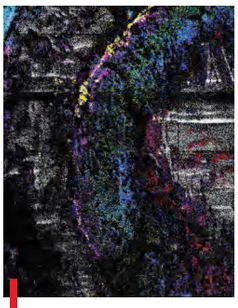
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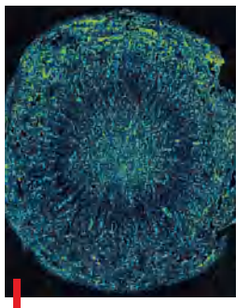
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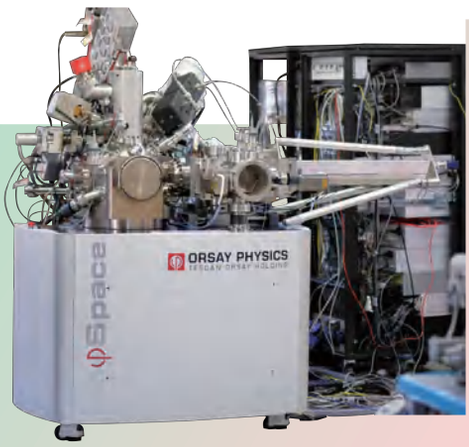


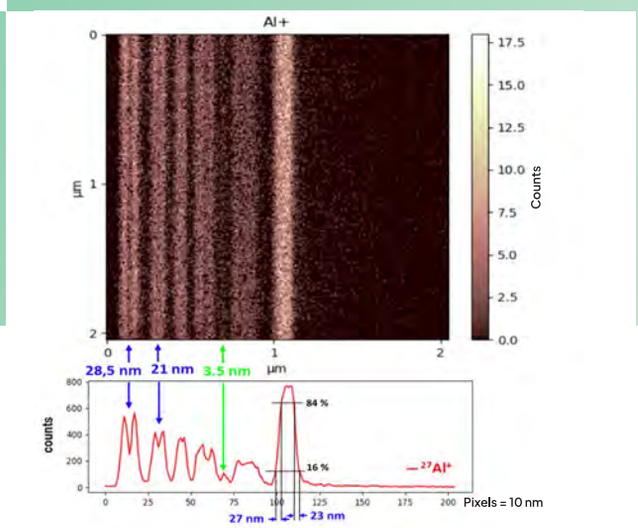
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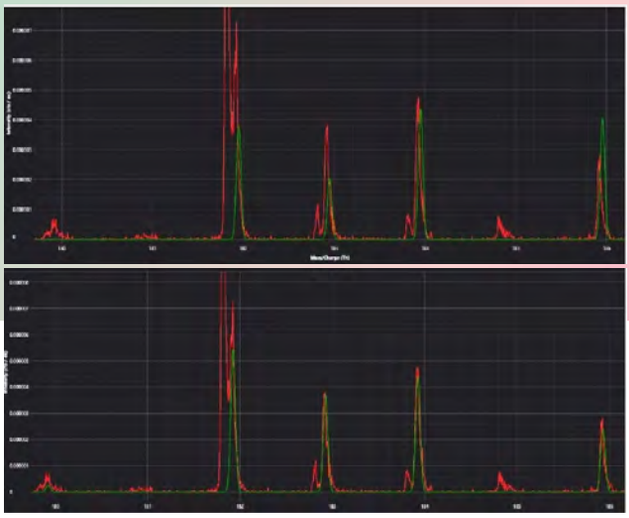
Nanospace with Tof-SIMS — FIB TOF

技术的巅峰之作





使用 NanoSpace 上的 OTOF-SIMS 对 BAML200 参考样本进行成像分辨率测量。空间分辨率达到 25nm（Ga离子源）。



红色谱峰是在 183-186 质量数实际测得的谱峰，上图绿色谱峰是 W 元素在此位置的同位素峰，下图绿色谱峰是 ErO+ 在此位置的同位素峰。经同位素丰度比和质量精度匹配，判断出这些质谱峰是氧化铒而不是钨。

相较于专用 SIMS 设备

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- 在一台设备上，SIMS 可以和 SEM、FIB、EDS、EBSD、AFM、XRF 等多种分析手段联用。
- Nanospace 可配置两个 FIB 镜筒和多种离子源选择（如 Ga/Xe/Ar/Au/Cs/O），提供了更广泛的可实现应用。

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- 六轴样品台允许在 SIMS 分析时，样品表面和二次离子提取镜筒呈 90°，将二次离子的提取效率优化到极致。

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- 光谱分析
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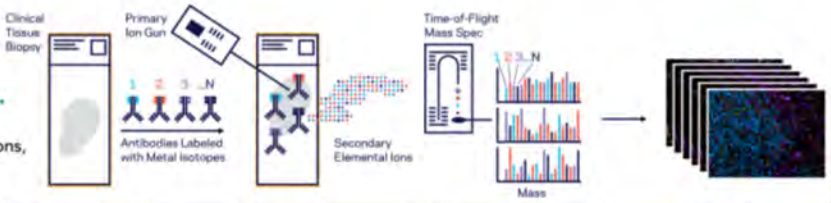
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质量精度 ±5 milli-amu



SurfaceSeer I · 高分辨率飞行时间二次离子质谱仪

离子束配置

- LMIG束斑尺寸最小可达50nm(连续模式)
- 25kV液态金属离子源(LMIG)

高品质设计

- 结构紧凑，适用于多种实验室
- 交错式扫描成像以实现均匀电荷分布
- 配备二次电子探测器（SED），用于样品成像

100~1000μm
分析区间

25 kV LMIG
一次离子束

技术规格

一次离子束	25 kV LMIG（可提供 Au、Bi、Ga 源）
溅射离子束	5 kV 氧、氩及铯离子束
灵敏度	~1×10^{9} atoms/cm^{2}
质量分辨率	>7,000 FWHM
质量范围	>1,000 amu
质量精度	±5 milli-amu
分析区域	100–1,000 μm
SIMS 模式	正 / 负离子模式下的成像分析
样本类型	导体和绝缘样品
分析时间	~1 min 起

应用场景

半导体　污染物分析　粘附性　印刷适性

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Fundamentals of SIMS – From nanocraters to gas phase ions

Arnaud Delcorte

Université catholique de Louvain, IMCN, 1 Pl. L. Pasteur, 1348 Louvain-la-Neuve, Belgium.

An initial particle impact on a surface – "big bang" in the universe of the SIMS aficionados – induces the generation of free gas phase ions which, after detection, constitute the secondary ion mass spectrum. It is the chemical signature of the sample "skin", of its topmost nanometer(s). While kiloelectronvolt monoatomic ion impacts and the subsequent emission of atoms could be reasonably described using analytical collision cascade theories (linear and spikes), quantitative predictions concerning energetic cluster-surface collisions and molecular emission largely relied on the progress of molecular dynamics computer simulations, and their ability to model increasingly large energies and system sizes as well as greater molecular complexity over the years (Fig. 1). In this short course, the basics of keV atom and cluster interactions with atomic and molecular solids are reviewed using the magnifying lens of the microscopic models. For instance, (large) cluster and molecular impacts differ radically from single atom impacts in that they systematically induce collective motions in the solid (pressure waves, correlated atomic and molecular motions, nanocrater formation), which make their action resemble (tiny) meteorite collisions [1]. The mechanisms of projectile penetration, energy deposition, atomic motion and damage in the solid in the first few picoseconds of the interaction are described. Beyond the impact, the emission of atoms, fragments and molecules are discussed, with an emphasis on the conditions of intact molecular emission as a function of the internal energy uptake and the projectile properties. Surface sensitivities are compared. Finally, the questions of ionization and matrix effects – annoying but so central to SIMS – are considered, and unresolved fundamental issues are delineated.

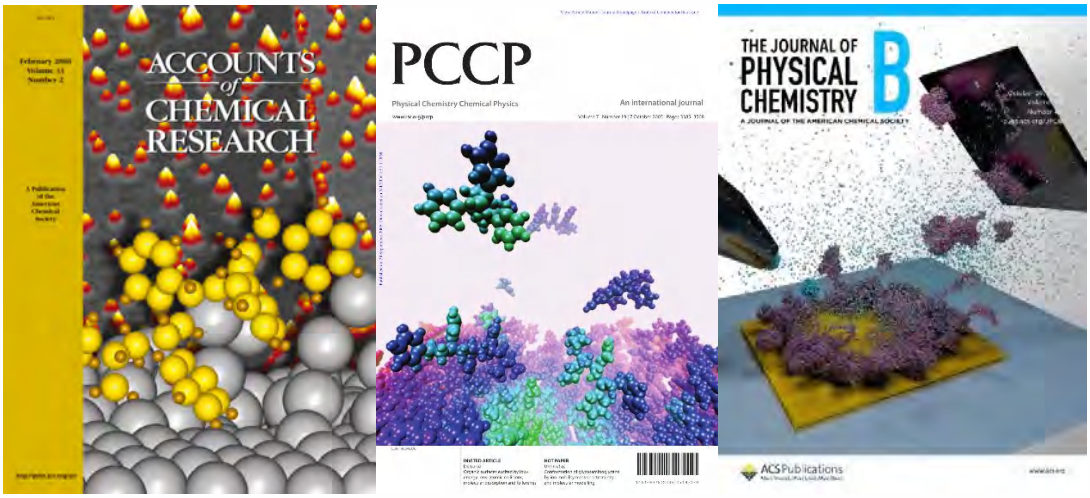


Figure 1. Views of the molecular dynamics from published articles. (A) Emission of polystyrene oligomers adsorbed on Ag induced by 500 eV Ar projectiles (2000). (B) Desorption from a bulk PS molecular solid under 5 keV Ar impact (2005). (C) Crater formation and molecular emission from an enzyme film bombarded by a 15 keV Ar_{5000} cluster (2023).

[1] A. Delcorte, B. Tomasetti and S. Bertolini, Cluster Ion Beams and Sputtering; Chap. 3 in: New Developments in Mass Spectrometry No. 16; Secondary Ion Mass Spectrometry: Fundamentals, Advancements and Applications, Ed. P. P. Michałowski; The Royal Society of Chemistry 2025. Pp. 93 – 132.

Electronics and 2D Materials: Leveraging SIMS Capabilities and Navigating Instrument Trade-offs

Paweł Piotr Michałowski[1]

(1) Łukasiewicz Research Network - Institute of Microelectronics and Photonics
al. Lotników 32/46, 02-668 Warsaw, Poland

Secondary Ion Mass Spectrometry (SIMS) is available in a wide variety of instrument configurations, including magnetic sector, time-of-flight, and quadrupole analyzers, employing different primary ion sources and increasingly complemented by advanced technologies such as Orbitrap mass analyzers or correlative approaches, including in situ AFM and glovebox integration. Each configuration offers unique strengths, while also introducing specific limitations that influence the type and quality of information that can be obtained.

As a result, researchers often perceive certain classes of materials or analytical problems as being accessible only with a particular SIMS instrument. For example, dynamic SIMS is commonly considered the preferred choice for hydrogen analysis, whereas ToF-SIMS is typically associated with organic and molecular characterization. Although such generalizations are often justified, they can also lead to unnecessary misconceptions. Many practical problems do not require the ultimate performance of a dedicated instrument, and valuable information can frequently be obtained using alternative SIMS platforms when their capabilities are properly understood.

This tutorial will present a systematic framework for evaluating SIMS capabilities for the characterization of electronic materials, devices, and two-dimensional materials. Key analytical parameters, including detection limits, mass resolution, lateral resolution, depth resolution, and quantification, will be discussed alongside practical challenges such as sample charging, non-planar surface morphology, ion-beam-induced material modification, preferential sputtering, and matrix effects. Particular emphasis will be placed on understanding which limitations are fundamental and which can be mitigated through thoughtful experimental design, optimized measurement conditions, or a reformulation of the analytical question.

Rather than focusing on the superiority of individual instrument designs, the tutorial aims to provide participants with a practical strategy for selecting the most informative measurement approach for the available instrumentation. The objective is to help researchers recognize both the capabilities and the limitations of their SIMS platform, enabling them to extract the maximum meaningful information from challenging electronic and two-dimensional material systems.

Applications of NanoSIMS in Biological Materials

Katie L. Moore[1]

(1) Department of Materials, The University of Manchester, Manchester, UK

The NanoSIMS enables high spatial resolution elemental and isotopic imaging (down to 50 nm), with high sensitivity, making it ideally suited for subcellular localisation of elements and isotopic tracers in biological materials.

In this presentation, I will show how NanoSIMS can be applied to a range of biological samples. Examples will illustrate how elements of interest can be correlated to other signals to understand elemental uptake or storage mechanisms and how stable isotopes can be used in pulse-chase experiments which can provide temporal information about uptake and metabolism.

The analysis of biological samples with the NanoSIMS, which operates under ultra-high vacuum, is complicated by the need to preserve not only the in-vivo structure of the cellular components but also the elemental distribution. This presentation will outline the two main approaches for sample preparation, chemical or cryo fixation, and how the choice depends on the biological question or the size of the sample. In all cases the ideal sample preparation methodology workflow is fixation, dehydration, resin embedding and microtomy to create a sample that is flat and high-vacuum compatible. Sample preparation methods will be discussed in the context of the examples presented.

In this presentation I will show case studies of how we have used the NanoSIMS to analyse a range of biological materials ranging from trace element uptake in plants and algae, use of isotopic labelling to investigate the feeding mechanism of the whipworm parasite, the analysis of bacteria and nanoparticle distributions in plants and algae. Throughout my presentation I will show how we have used complementary and correlative imaging and how it fits into the broader analytical workflow to gain a deeper understanding of the samples than could be obtained from one technique alone.

How machine learning can improve your interpretation of SIMS data

Satoka Aoyagi[1]

(1) Faculty of Science and Technology, Seikei University, 3-3-1 Kichijoji-kitamachi, Musashino, Tokyo

Machine learning [1-4] can be powerful for extracting information from complex datasets. In order to apply machine learning effectively to our datasets, we first need to understand what they are. Unsupervised learning methods are helpful in providing an outline of a target dataset, after which supervised learning methods can be applied to extract particular information that is needed. The application of machine learning can also reveal how complex but rich information secondary ion mass spectrometry (SIMS) datasets have. Even extremely complex datasets can be interpreted more easily if they are classified into simpler categories. Moreover, if the classified ones are still difficult to understand, mass peaks can be identified by using supervised learning methods.

In terms of identifying organic materials, we now have more options, such as time-of-flight mass spectrometry, tandem MS (MSMS) and Orbitrap. MSMS spectra can be compared with conventional databases, and many precisely identified mass peaks can be matched to those in mass spectrometry databases. Therefore, the interaction between conventional databases and mass peaks in acquired SIMS spectra will be as important as it is to mass spectrometry fields. Understanding the fundamental mechanisms of machine learning is crucial for every SIMS researcher to effectively deal with complex datasets.

This tutorial will introduce the history of machine learning applications to SIMS datasets, the principles of basic machine learning methods, and several applications. Machine learning is generally classified into three types: unsupervised, supervised, and reinforcement learning. Unsupervised learning methods such as principal component analysis (PCA) and non-negative matrix factorisation (NMF) are commonly used to extract important features from a sample. Furthermore, artificial neural network (ANN) based methods such as autoencoders and self-organising maps are effective for analysing datasets containing nonlinear factors, such as matrix effects [1-3]. Correction of matrix effects is essential for quantitative analysis, as well as for obtaining appropriate mass images. ANN-based methods can be used effectively once the basic structures of ANNs have been understood. Therefore, the material that is useful for understanding perceptron and multilayer perceptron will be shared. Applications of supervised learning systems developed through the Versailles Project on Advanced Materials and Standards (VAMAS) will then be introduced, including quantitative and qualitative analyses of organic SIMS data using an ANN-based supervised learning method (VAMAS TWA2 A31) [3] and a material prediction system using a Random Forest-based supervised learning method developed by extending the peptide prediction system (VAMAS TWA2 A26) [4]. Furthermore, Python codes and Excel files for practical use will be shared.

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Cryogenic Atom Probe Tomography: Expanding the Frontiers of Atomic-Scale Materials Characterization

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Atom probe tomography (APT) enables three-dimensional compositional analysis of materials with near-atomic resolution and, in principle, allows the detection of all elements, including hydrogen. However, accurate characterization of hydrogen and its isotopes using conventional APT remains challenging. During specimen preparation and transfer through ambient conditions, samples are highly susceptible to hydrogen contamination, while residual hydrogen in the analysis chamber contributes additional background signals. In addition, hydrogen exhibits extremely high mobility at room temperature and can rapidly diffuse out of the nanoscale needle-shaped APT specimens, making it difficult to preserve its intrinsic distribution within materials.

To address these challenges, cryogenic atom probe tomography (Cryo-APT) has recently been developed by integrating ultrahigh-vacuum and cryogenic specimen handling with the conventional APT workflow. In this approach, samples are maintained at liquid-nitrogen temperature under ultrahigh-vacuum conditions throughout preparation and transfer between the preparation chamber and the atom probe instrument. These conditions effectively suppress external hydrogen contamination and significantly reduce hydrogen diffusion within materials, enabling improved preservation of their original atomic distributions.

Initial applications of Cryo-APT have emerged in studies of hydrogen embrittlement in metallic systems as well as in surface processes such as oxidation and corrosion. Looking ahead, Cryo-APT is expected to provide unprecedented atomic-scale insights into hydrogen storage materials, surface catalysis, and emerging energy materials such as batteries, opening new opportunities for exploring hydrogen-related phenomena in materials at the true atomic scale.

Exploring the Frontiers of SIMS: Pushing Forward Together

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The continuous evolution of Secondary Ion Mass Spectrometry (SIMS) has been driven by the synergy of innovative instrumentation and expanding application fields. Gas Cluster Ion Beams(GCIBs), originally developed for advanced material processing, have now become indispensable tools in cutting-edge semiconductor manufacturing. Thanks to the invaluable contributions of numerous collaborators, extending the application of GCIBs to surface analysis has brought about an unprecedented paradigm shift, opening up entirely new dimensions in molecular imaging and depth profiling.

Accurate molecular identification has long been a major challenge in SIMS, but recent innovations such as Orbitrap and MS/MS analyzers have dramatically improved this capability. However, the ultimate sensitivity remains strictly constrained by the secondary ion yield. Since a significant majority of sputtered species leave the surface as neutral particles, understanding their molecular structures is crucial for defining the theoretical limits of SIMS. Prior to the advent of GCIBs, it was believed that most sputtered organic molecules were fragmented during ion-collisions. In recent investigations, we successfully characterized the molecular structure of these neutral species using advanced capturing techniques.[1] Remarkably, a substantial fraction of the sputtered neutral particles actually remain entirely intact during the cluster ion bombardment. Quantitative measurements using polymer systems revealed that the survival rate—the ratio of unfragmented neutral molecules to total sputtered species—reaches several percent, though it gradually scales down with increasing molecular weight.

These findings unveil a profound opportunity: if these abundant, intact neutral particles can be efficiently post-ionized, the secondary ion yield could be boosted by several orders of magnitude. Although implementing an optimal post-ionization framework within advanced mass spectrometers is a highly challenging subject, drawing inspiration from related disciplines like MALDI-2 suggests that breakthroughs are within reach. Pushing the frontiers of SIMS requires collective exploration into novel ionization methodologies, paving the way toward ultimate sensitivity together.

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Pore-confined ToF-SIMS electrochemistry

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Electrode-electrolyte interfaces govern charge transfer, mass transport, solvation, adsorption, and structural evolution in electrochemical energy systems. However, the dynamic molecular processes remain difficult to probe under operando conditions. Pore confined time-of-flight secondary ion electrochemical mass spectrometry integrates ToF-SIMS with a vacuum-compatible electrochemical microfluidic cell, enabling direct interrogation of liquid electrochemical interfaces under operando conditions. By stabilizing a nanoscale liquid-vacuum interface within a confined aperture, this strategy enables real-time acquisition of mass-resolved molecular information from the electrode surface during electrochemical reactions. With high surface sensitivity, mass resolution, and spatiotemporal resolution, this technique enables the identification of transient intermediates, reaction products, solvated species, spectator ions, and electric-double-layer evolution. Representative studies demonstrate its capability to probe molecular transformations, proton-coupled electron transfer, ion-solvent interactions, electrocatalytic pathways, and solid-electrolyte interphase formation in battery systems. This presentation will highlight the working principle, analytical capability, and representative applications of pore confined ToF-SIEMS, while outlining current challenges in device design, vacuum stability, interfacial sampling, and quantitative interpretation, as well as future opportunities in electrochemistry, energy conversion, bioanalysis, and chemical sensing.

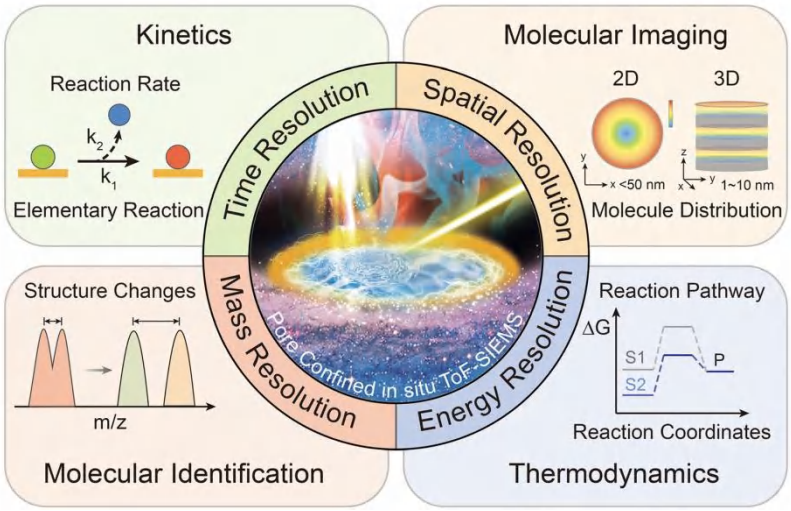


Figure 1. Concept of ToF-SIEMS probing the EEIs through the pore confined configuration.

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Development of a new system for multimodal ion beam imaging using keV and MeV ion beams

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We describe the design of a unique new system for multimodal ion beam imaging by using both MeV and keV ion beams in a single system. The equipment, due to be installed and commissioned in May 2026, will enable multimodal mass spectrometry and MeV Ion Beam Analysis (IBA) analysis, to provide a comprehensive analysis of metals, lipids, metabolites, proteins and other molecules at high spatial resolution.

To do this, we are using a commercially available system for secondary ion mass spectrometry (SIMS), in which ion transport and detection is already optimised. This system uses gas and water cluster keV ion beams, which have recently been shown to provide enhanced coverage of organic molecules in comparison to other primary ion beams used in SIMS. The system will be integrated with the 2MV Tandem accelerator at the University of Surrey, using the MeV ion beam as an alternative primary ion beam. The analysis chamber will include detectors for particle induced X-ray emission (PIXE), Rutherford backscattering spectrometry (RBS) as well as a quadrupole-ToF detector for tandem mass spectrometry analysis. The new system is designed to enable the following:

* MeV-SIMS using optimised secondary ion detection and MS/MS capability to enable speciation analysis of biological molecules
* Multimodal gas cluster SIMS and PIXE, for the co-localization of trace elements (PIXE) and lipids/ metabolites
* Multimodal keV-SIMS and MeV-SIMS, to enhance the coverage of molecular species
* Multimodal depth profiling using MeV (RBS) and keV (SIMS) beams to provide depth profiles of inorganic and organic constituents
* Cryogenic stage to enable analysis of frozen hydrated specimens

The presentation will summarise the key technical features of the system, design considerations and plans for future work.

Acknowledgements

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Key words: MeV-SIMS, Cluster SIMS, PIXE, MeV Ion Beam Analysis, Multimodal Imaging

Establishing the Static Limit for Organic Materials in Combined MeV SIMS and PIXE Analysis

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Secondary Ion Mass Spectrometry with MeV energy ion beams (MeV SIMS) is a well-established technique for characterizing organic materials, routinely employed for over a decade at the Ruđer Bošković Institute. MeV SIMS enables molecular identification of compounds up to ~1000 Da and, when combined with a focused ion beam, allows for two-dimensional mapping of molecular distributions with micrometer lateral resolution. Because MeV SIMS cannot provide elemental data, it is often complemented by Particle Induced X-ray Emission (PIXE). However, combining these techniques presents a challenge: PIXE requires ion fluences approximately six orders of magnitude higher than the low fluences used in MeV SIMS. Relatively little is known about how such high-current irradiation affects organic sample integrity prior to MeV SIMS analysis.

In this study, the effect of ion fluence on molecular yield was investigated by measuring secondary ion signals as a function of incident heavy ion fluence. The aim was to determine the damage cross-sections and identify the static SIMS limit. The damage cross-sections for leucine, cholesterol, phthalocyanine, and a real paint sample were measured using 5 MeV Si^{4+} and 9 MeV O^{4+} ion beams. We performed initial pulsed-mode measurements on pristine surfaces, followed by high-current irradiation at 10^8 – 10^9 ions/cm². By monitoring beam currents via a PIN diode, we tracked changes in the yield of intact molecular and fragment ions. We conclude by discussing the damage cross-sections determined for these materials and their implications for analytical workflows.

Correlative Imaging of key 2D materials with SIMS, AFM and SEM

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Advances in the exploration of two-dimensional (2D) materials have accelerated significantly since the discovery of graphene in 2004. Subsequently, other 2D materials such as black phosphorus and molybdenum disulfide have been identified and extensively studied. As research in this field has progressed, the associated analytical challenges have increased. Surface-sensitive analytical techniques are particularly well suited to address the diverse characterization requirements.

Scanning electron microscopy (SEM) and atomic force microscopy (AFM) provide valuable information on the morphology and topography of these materials, whereas techniques such as secondary ion mass spectrometry (SIMS), energy-dispersive X-ray spectroscopy (EDS), and Auger electron spectroscopy (AES) offer detailed insights into surface and near-surface chemistry. However, each of these techniques has inherent limitations. Consequently, a correlative, multi-technique approach is often required to obtain a comprehensive understanding.

In this study[1], the performance of SIMS, EDS, and AES was compared. In addition, functionalized graphene flakes embedded in a complex carbon-based ink matrix were successfully identified using a combined SIMS-SEM approach (Figure 1a). Metal impurities originating from the production process were also detected on the graphene flakes within these matrices. Notably, the spatial distributions of different metals varied. For example, the distribution of Al^+ ions correlated with that of O^- ions, whereas Fe^+ ions co-localized with F^- ions (Figure 1b).

Furthermore, either as a standalone technique or in combination with AFM, SIMS proved to be a highly effective tool for the analysis of 2D materials.[2]

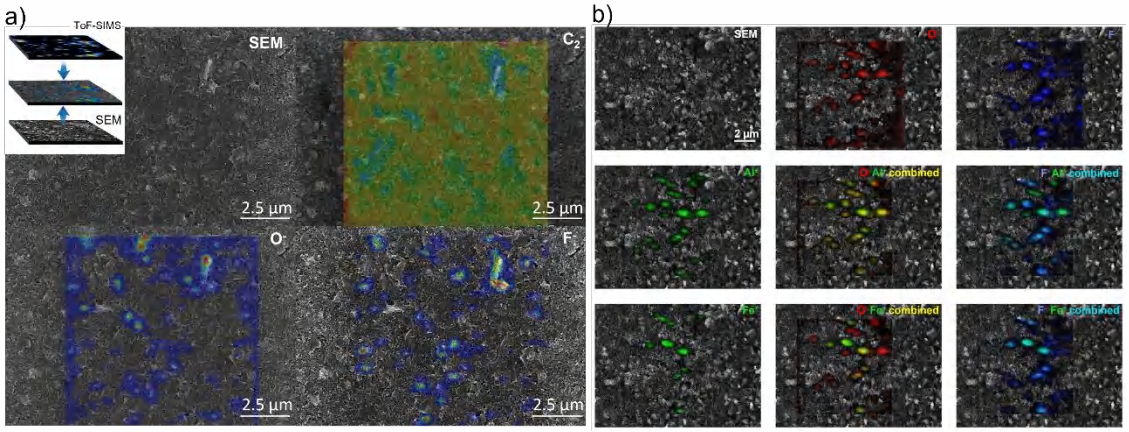


Figure 1. a) SIMS negative mode images on SEM image of a complex carbon-based matrix consisting of functionalized graphene flakes and carbon black (inset illustrates the idea of correlative analysis) and b) metal impurities and their overlapping in position with F^- and O^- fragments in the same matrices.

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Data Analysis for Biological SIMS Research

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Biological analysis using SIMS has increased in recent years along with the capabilities of SIMS instruments. The spectral quality, in terms of mass resolution and mass accuracy, has improved [1-3] which in turn facilitate computational based analysis and directly impact peak identification/assignment. Complementing the spectrometer improvements, ion beam developments, specifically the introduction of gas cluster ion beams (GCIBs)[4] has greatly improved the ability to detect intact biomolecules. Hence, our expectations from a biological SIMS experiment have changed significantly. As have the challenges and so, and also the opportunities, for exploiting the information that is sometimes quite well hidden in the increasingly complex SIMS data.

This presentation will discuss these challenges and opportunities with reference to studies of cultured cells and tissue section samples including data reduction, classification and spectral interpretation.

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A Better File Format for SIMS Data

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FAIRSpectra (https://fairspectra.net/) is a community-driven initiative to improve data management and sharing, with particular focus on spatial spectrometries and spectroscopies.

The FAIR Guiding Principles approach to research data – that data should be Findable, Accessible, Interoperable and Reusable – were developed in 2016, and much activity is taking place around the world in this area [1,2].

FAIRSpectra are mostly engaged with how to make our data Interoperable: how different software systems can read our files, and understand the sample, experiment, instrumentation, and any data processing steps used.

Unfortunately, FAIR is often confused with OPEN, with people assuming that if their data conforms to the FAIR Principles, it must be shared openly. This is not the case. FAIR approaches can be hugely beneficial in a CLOSED environment; for example, within a business. Freely available tools can be used to document in-house processes and outcomes, without the need to make those data public. This leads to better internal records-keeping, and better data transfer mechanisms to move data between departments and sites. Acquisitions and mergers become more straightforward, and new staff can 'hit the ground running' if they are already familiar with FAIR approaches and methods.

One of the FAIRSpectra activities considers SIMS data: in particular, data from hyperspectral imaging experiments. Here, there are two related deliverables: appropriate information (metadata) to describe the experiment; and a suitable encoding of the data for modern cloud- and AI-friendly use. A further step envisions the concept of a minimum reporting requirement for our data.

In this presentation we will share the status of these projects, and how you can get involved to shape the outcomes.

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Decoding Human Hair Treatments via Hierarchical Molecular Attribution

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Secondary Ion Mass Spectrometry (SIMS) possesses excellent surface sensitivity for nanoscale, in situ analysis of chemical dynamics at complex biological interfaces [1~3]. However, the mechanistic interpretation is often obscured by matrix effects, fragmentation and persistent siloxane-like or inorganic backgrounds. Here, using damaged keratin fibers treated with haircare products, which contain typical haircare active ingredients (α-hydroxy acids, cationic surfactants), we report a background-aware, hierarchical molecular attribution strategy for cryogenic Hybrid SIMS analysis. Based on a hierarchical Nonnegative Matrix Factorization (NMF) algorithm using Kullback–Leibler (KL) divergence, ToF-SIMS and Orbitrap data can be decomposed into Background (contamination), Shared (hair matrix), and Local (specific ion families indicating the haircare mechanism) parts. Rather than removing contamination signals, the model assigns them to explicit background roles, separating salt and siloxane signals from treatment ions and revealing depth patterns linked to cryogenic fragment preservation, chelation and ionic rebinding. The approach improves the mechanistic readability of Hybrid SIMS analysis and provides a powerful route to distinguish background chemistry, structural damage characteristics and targeted chemical interactions in complex biological materials.

Acknowledgement
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Machine learning for individual extracellular vesicle classification based on highly sensitive multiplexed SIMS measurements

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Extracellular vesicles (EVs) are nano-sized, lipid membrane-bound particles secreted by cells into various bodily fluids. They carry molecular markers related to their cellular origin and pathological state, making them promising candidates for disease detection. However, a major challenge in using EVs for diagnositic purposes in a clinical setting is EV heterogeneity. Patient samples will contain Evs from multiple sources and even EVs arrising from the same tissue will contain different markers and have varied marker abudnance. Analyzing EVs at the single-particle level enables the distinction between EVs from diseased and healthy cells within complex biological samples. To examine individual EVs we employed Nano-Projectile Secondary Ion Mass Spectrometry (NP-SIMS), a technique in which individual projectiles are temporally and spatially separated, each sampling a nano-volume approximately 10 nm in diameter. In this mode, millions of mass spectra are collected, with each spectrum corresponding to a single EV. This approach allows for EV-by-EV analysis, thereby avoiding ensemble averaging. The remaining challenge lies in accurately classifying each EV based on its individual mass spectrum. Here, we developed a Random Forest (RF) model to classify EVs one by one using the single mass spectrum obtained by NP-SIMS. We trained our initial RF model on isolated EV samples derived from HEPG2 cells and normal cells. We benchmarked the RF model by comparing it to previously published results obtained by manual analysis of a 1:1 mixture of HEPG2 and normal EVs and found good agreement between the manual method and the results obtained from the trained RF. We found that improving the data preprocessing was critical for the performance of the model and after optimization we found a 60-fold improvement in EV classification using a RF model compared to manual inspection. We attribute 8-fold of this improvement to changes in the method of EV classification and 8-fold directly to the use of the RF. Further, we evaluated supervised and unsupervised RF models and found that both methods were compatible with NP-SIMS and the results were in good agreement with the manual analysis approach. Lastly, we examined the possibility of combined RF and NP-SIMS for untargeted analysis of EVs. Overall, we demonstrate that the RF combined with NP-SIMS is capable of classifying individual EVs from a 1:1 mixture of healthy and cancer EVs, and this is a promising method for disease diagnosis. These findings suggest that using machine learning, particularly RF, can significantly enhance NP-SIMS sensitivity and allow for rapid EV classification. This project is supported by the National Institutes of Health R01 DK134661.

Key words: Extracellular Vesicles, Random Forest

SIMS analysis of hydrogen in nominally anhydrous minerals (NAMs): Technical Challenges and Implications

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Numerous studies in the past three decades have demonstrated that nominally anhydrous minerals (NAMs) -- such as olivine, pyroxene, plagioclase, and garnet -- can contain from a few to hundreds of parts per million (ppm) water, mainly as structurally bound OH. These discoveries fundamentally changed the view that major mantle minerals are "dry" and established NAMs as important reservoirs and carriers of water in planetary interiors [e.g., 1-4]. SIMS has played a critical role in detecting and measuring such low water abundances because of its high sensitivity, micrometer-scale spatial resolution, and ability to analyze zoned or inclusion-rich samples *in situ* [5-7]. This presentation discusses the analytical challenges and caveats inherently associated with SIMS analysis of water in NAMs, and highlights its broad implications for geosciences.

There are five important aspects that must be carefully addressed when measuring extremely low water contents in NAMs by SIMS: (1) sample preparation; (2) sample residence time in vacuum; (3) instrumental and analytical conditions; (4) standard selection and calibration strategy; and (5) examination and selection of targeting spot during analysis. To achieve the lowest detection limits and the most accurate results, all these factors must be optimized.

SIMS analysis of water in NAMs has yielded broad and significant implications in geosciences. It has led to major re-evaluations of its mantle water budget, mantle rheology, melting behavior, and volatile recycling through subduction [2-4]. For planetary materials, SIMS analysis of NAMs, in addition to apatite and melt inclusions, has shown that the Moon is not completely dry, but retains indigenous magmatic water, providing new perspectives on lunar origin and differentiation [8-10]. Comparable analyses of NAMs in Martian meteorites indicate that Mars possessed heterogeneous mantle reservoirs containing water and other volatiles, with later exchange among mantle-derived magmas, crust, and atmosphere [11-12]. In primitive asteroids and differentiated parent bodies, water in NAMs provide constraints on accretion, thermal metamorphism, aqueous alteration, and volatile retention during early Solar System evolution [13]. Continued improvements in SIMS analytical techniques will advance our understanding of water and other volatile inventories in rocky planets and asteroids.

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High-precision SIMS Pb-Pb dating of Niobium Mineralization at Bayan Obo Deposit

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Abstract Content:

Matrix-matched calibration by external standardization of well-characterized natural references is a principal requirement for precise SIMS U-Pb age determination for U-bearing minerals (such as zircon). However, this matrix-matched calibration strategy is not applicable for dating minerals with complex chemical compositions such as zirconolite (ABC_2O_7; A = Ca, REE, Na, U, Th; B = Zr; C = Ti, Fe, Nb, Al, Mg) and aeschynite (ABO_7; A = REE, Ca, Fe, Th, U; B = Ti, Nb). Alternatively, the chemically-complex minerals (with a closed U-Pb system) can be dated by measurement of $^{207}Pb/^{206}Pb$ isotopic ratio, i.e., Pb-Pb dating method, without external standardization. Due to the low abundance of ^{235}U, the main challenge in SIMS Pb-Pb dating method is to precisely determine the age of young minerals (<1000 Ma). During the past decade, we have developed high-precision SIMS Pb-Pb dating method using the multicollector SIMS mode, which can precisely dating various U-bearing minerals as young as ~200 Ma . And this method has been successfully applied to determine the age of major Nb mineralization at the Bayan Obo deposit.

The Bayan Obo deposit in China is the world's largest REE deposit and also represents one of the most significant Nb endowments. Despite decades of study, the timing and genesis of Nb mineralization at the Bayan Obo deposit remain poorly constrained. This is due to the deposit's complex, multistage geological evolution spanning over one billion years and the presence of more than 30 Nb minerals. To reconstruct the temporal framework of Nb mineralization, we carried out systematic SIMS Pb-Pb dating of aeschynite, which is the most important Nb mineral accounting for >30% of the Nb resource of the deposit[2]. Thirteen aeschynite samples from various ore types were selected for SIMS Pb–Pb dating. Among them, 11 samples yield consistent ages between 402 ± 43 and 449 ± 56 Ma, with a weighted mean of 429 ± 11 Ma[3]. The remaining two aeschynite samples yield ages of ~270 Ma[3, 4]. Our new aeschynite ages, in combination with published geochronological data, indicate that the principal Nb mineralization at Bayan Odo occurred in the early Paleozoic, coincident with the newly identified ~430 Ma carbonatite dikes throughout the mining area[5]. The Nb mineralization is most likely controlled by carbonatite-derived hydrothermal fluids. The pre-existing Nb mineralization was locally reworked or remobilized by regional Permian (~270 Ma) granite plutonism[3, 4].

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Key words: SIMS Pb-Pb dating; multicollector SIMS mode; aeschynite; Nb mineralization; Bayan Obo

Presolar Grain Research Via High-Resolution nanoSIMS Isotopic Imaging

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Introduction: Presolar grains are submicron- to micron-sized dust particles that formed in stellar outflows and explosions before the birth of our solar system. As *bona fide* stellar material, they provide unique insights into astrophysical and cosmochemical processes with precisions surpassing astronomical observations [1]. However, their original stellar signatures are often diluted by exogenous material concentrated at grain surfaces. The development of the Hyperion-II radio-frequency plasma oxygen ion source in 2016 [2] enabled isotope analyses (e.g., titanium) via nanoSIMS at improved spatial resolution (i.e., ~100 nm), allowing selective data acquisition from grain interiors during analysis and excluding contaminated surface regions. Here, we summarize key advances in presolar grain research achieved in recent years using the Carnegie Hyperion-nanoSIMS microprobe.

Resolving Radiogenic vs. Nucleosynthetic Anomalies: Presolar grains exhibit excesses in ^{26}Mg, ^{41}K, and ^{44}Ca, which may originate from either *in situ* decay of ^{26}Al ($t_{1/2}$ = 0.72 Ma), ^{41}Ca (0.1 Ma), and ^{44}Ti (60 a), respectively, or direct stellar nucleosynthesis processes such as neutron capture. Distinguishing these mechanisms is critical for constraining their stellar origins and nucleosynthesis in parent stars. Using Hyperion-NanoSIMS isotope imaging at ~100 nm resolution, we observed (*i*) spatially correlated ^{26}Mg excess with ^{27}Al in different presolar grain groups [3, 4], (*ii*) spatially correlated ^{44}Ca excess with ^{48}Ti in a Type-X (enabling derivation of its initial ^{44}Ti/^{48}Ti ratio and nonradiogenic ^{44}Ca excess, Fig. 1) and Type-AB SiC grain [5, 6], and (*iii*) spatially correlated ^{41}K excess with ^{40}Ca in three supernova-origin Si_3N_4 grains. These spatial correlations confirm the initial incorporation of ^{26}Al, ^{41}Ca, and ^{44}Ti and allowed for more accurate deveriation of their initial isotopic ratios. In addition, the improved spatial resolution led to the discovery of ^{63}Cu excesses (likely resulting from the decay of ^{63}Ni with $t_{1/2}$ = 100 a) in two X and one C SiC grain by mitigating copper contamination. The inferred initial ^{63}Ni/^{58}Ni ratios provide important constraints on the neutron-burst process during supernova explosions [7].

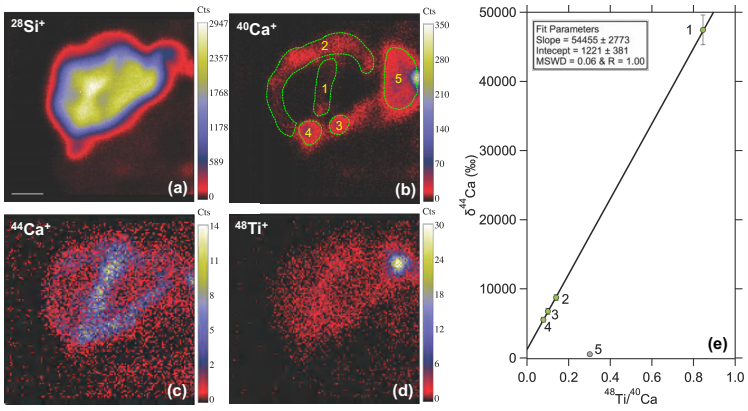


Figure 1. *Panels (a) to (d) show the ^{28}Si, ^{40}Ca, ^{44}Ca, and ^{48}Ti ion images of an X grain. The white scale bar in panel (a) denotes 500 nm. In panel (b), different regions of interest (ROIs) were defined for reducing the Ca-Ti isotope data in panel (e). Errors are all 1σ. The data for ROI #5 was excluded from the linear fit because of its significant deviation (Adapted from [5]).*

Suppressing Isobaric Interferences: High spatial resolution (~100 nm) in Hyperion-NanoSIMS imaging further mitigates isobaric interferences by enabling selective analysis of grain interiors during data reduction. For example, presolar SiC grains are intrinsically enriched in titanium and nickel but often exhibit surface contamination from chromium and zinc. At mass 50, ^{50}Cr can obscure ^{50}Ti signals, while at mass 64, ^{64}Zn overlaps with ^{64}Ni. By targeting small, less-contaminated regions within grains, contributions from chromium and zinc (predominantly at edges) are minimized, yielding more accurate measurements of ^{50}Ti and ^{64}Ni — the most neutron-rich isotopes of their elements, whose abundances are highly sensitive to neutron exposure. Using this approach, we reliably extracted correlated ^{50}Ti/^{48}Ti and ^{64}Ni/^{58}Ni ratios from both AGB and supernova SiC grains [7, 8]. These data provide stringent constraints on the *s*-process in AGB stars and neutron-burst nucleosynthesis in supernovae.

Conclusions: The Hyperion-nanoSIMS microprobe, with its unprecedented ~100 nm spatial resolution, has revolutionized presolar grain studies. By preserving pristine stellar signatures while suppressing external contamination, this technique continues to unlock novel astrophysical and cosmochemical insights from microscopic stardust.

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U-Pb Detrital Zircon Geochronology of Fluvial Sediments in North-Central Iceland

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Iceland provides a unique setting for investigating divergent plate- boundary processes in a subaerial environment, driven by the interaction between the Mid-Atlantic Ridge and the Iceland Plume. Eyjafjarðará in the north-central Iceland cuts through Neogene flood basalts and silicic rocks of the fossil Torfufell Central Volcano (ToCV). Activity of the ToCV at approximately 6.8 - 7.2 Ma coincided with a major phase of tectonic reorganization, during which the rift axis shifted from the Snæfellsnes-Húnaflói Rift Zone (SHRZ) toward the present-day Northern Volcanic Zone (NVZ) [1]. This area therefore preserves an important record of rift-zone migration linked to plume motion. This work presents and initial geochronological investigation of fluvial sediment samples collected along Eyjafjarðará river profile.

Of the seven collected sediment samples, four yielded zircon grains that were dated by U-Pb secondary ion mass spectrometry (SIMS). A total of 41 zircon analyses yielded $^{206}Pb/^{238}U$ ages between 5.1 and 8.2 Ma. Three samples yielded weighted mean ages of 7.18 ± 0.12 Ma (n = 18), 7.48 ± 0.23 Ma (n = 5), and 7.39 ± 0.44 Ma (n = 2), consistent with the documented active phase of the ToCV at 6.76–7.15 Ma. These results support the interpretation of the ToCV as the dominant zircon source for the studied sediments [2]. In addition, one sample contains a younger zircon population dated with an age of 5.3 ± 0.2 Ma (MSWD = 0.83, n = 3), which may indicate sedimentary input from the neighboring Tinná Central Volcano (TiCV). Overall, the detrital zircon data support previously established age constraints and are consistent with the westward migration of silicic magmatic activity along a proposed “leaky transform zone” during Late Miocene rift migration in northern Iceland.

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Beyond the Coating: How Glass Chemistry Drives Adhesion

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What determines how well coatings adhere to glass, and why does adhesion change over time? To answer these questions, we must look beyond coating formulations and recognize glass itself as an active player in adhesion. By leveraging ToF-SIMS and other analytical tools to examine the chemistry on both sides of the adhesion equation (coatings and glass), we uncover how subtle variations in glass composition trigger chemical interactions and degradation of the film, particularly over extended periods at elevated temperature and humidity. Through examples—including model ink coatings with silanes that promote stronger adhesion and polyolefin-based film laminates, which are largely governed by van der Waals forces—we demonstrate how detailed analysis of the glass–coating interphase can expose root causes of failure that are often overlooked in conventional adhesion science. These insights highlight the value of chemically resolved interfacial analysis for understanding, predicting, and ultimately improving the durability of glass–organic interfaces.

Figure 1 shows an example of ToF-SIMS assessment of a model ink coating on soda-lime glass before and after accelerated aging. The analysis reveals significant alkali migration into the coating, and accumulation of alkali reaction products at the coating/glass interface, providing direct insight into the chemical processes that contribute to adhesion loss. As will be discussed, the migration of sodium-containing species into the coating can promote coating degradation, further influencing adhesion. Although multiple tools were used in this study, ToF-SIMS is particularly powerful because it enables characterization of all interfaces while providing 3-D chemical information from both the glass and coating sides.

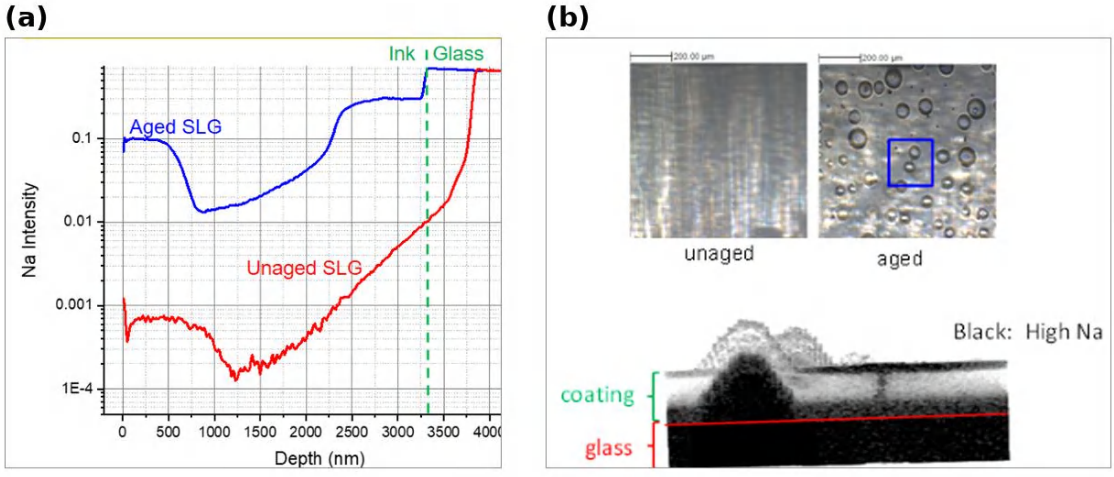


Figure 1. (a) ToF-SIMS depth profiles of a model ink coating on unaged and aged soda-lime glass: after aging (85 °C, 85% RH, 500 h) considerable sodium migration is observed into the coating. (b) Optical images of the coating before and after aging, together with a 3-D ToF-SIMS reconstruction, reveal that the migrated sodium forms sodium-rich corrosion products and pinhole defects localized precisely at the coating/glass interface—the sites where adhesion ultimately fails.

TOF-SIMS ^{2}H isotope Distribution Analysis of Mechanically Induced Cracks in Soda-Lime Glass

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Numerous studies and experiments have demonstrated the significant influence of water and humidity on crack growth in various types of glass [1] [2] [3]. Hydrogen significantly influences crack growth in glass under mechanical stress while promoting crack-tip healing in stress-free conditions, though underlying mechanisms remain unclear. Here, we investigate water-glass interactions at crack tips in soda-lime silicate glass using high-resolution Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS).

Cracks were generated via Vickers indentation and conventional glass cutting, then exposed to ambient conditions, heavy water ($^{2}H_2O$), or deionized water to simulate weathering. ToF-SIMS (IONTOF M6 Plus, equipped with FIB) enabled elemental mapping of ^{1}H and ^{2}H, revealing species distributions at crack interfaces and at FIB-cut cross-sections.

Our findings provide new insights into the role of Hydrogen mobility in glass cracks, potentially improving our understanding of crack propagation and healing mechanisms at the sub-micrometer scale.

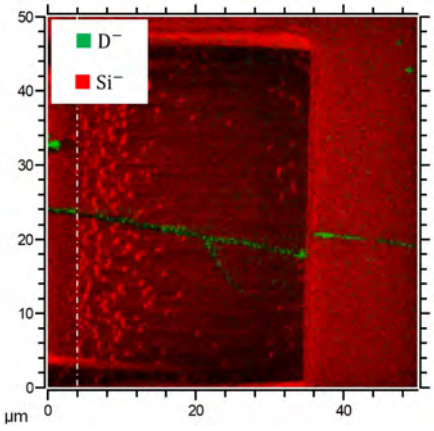


Figure 1. ToF-SIMS image overlay of Deuterium (green) and Silicon (red) in negative ion detection mode of a FIB crater on a crack that was stored in a container with heavy water for 14 days; Instrument: M6 Plus

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Cryo Q-SIMS for Reliable Depth Profiling of Alkali Ions in SiO_2

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Alkali ion migration in SiO_2 during secondary ion mass spectrometry (SIMS) analysis is a well-recognized issue that can significantly distort depth profiles. Na^+ ions exhibit high mobility under ion bombardment and tend to redistribute toward surfaces or interfaces due to internal electric fields and local temperature increases, leading to artificial surface enrichment [1].

Low-temperature SIMS (cryo-SIMS) has been shown to effectively suppress this migration and improve depth profiling accuracy [2,3]. It should be noted that Refs. [2] and [3] are based on time-of-flight SIMS (ToF-SIMS), which provides high mass resolution and surface sensitivity, whereas quadrupole SIMS (Q-SIMS) is more suitable for quantitative depth profiling due to its higher dynamic range and stable sputtering conditions. Nevertheless, the underlying migration mechanisms are common across SIMS techniques.

Additionally, charge compensation using an electron flood gun can modify the local electric field and further enhance Na^+ migration, making precise control of temperature and charge compensation essential.

In this study, Q-SIMS instrument (PHI ADEPT, ULVAC-PHI) equipped with a hot/cold stage was used to perform in-situ cooling below −110 °C, effectively suppressing ion migration and improving depth profiling reliability.

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Key words： cryo-SIMS,Q-SIMS , PHI ADEPT

Enabling TOF-SIMS based correlative analysis with novel sample preparation and data treatment

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The high sensitivity, detection of elements and molecules and relatively good lateral resolution of time-of-flight mass spectrometry imaging has been exploited in many applications ranging from microelectronics to biology. However, it does suffer from limitations and artefacts that can be overcome by using correlative approaches. These can be used to improve quantification, add new information such as physical or electrical properties, correct sputter rate variations in 3D imaging, or supply higher resolution images of the same sample area.
For example, argon cluster sputtering can be used to generate wedge craters of OLED stacks that allows correlative TOF-SIMS and XPS analysis on exactly the same area with so little damage that this method may be used to characterise the degradation in the layers in order to understand device degradation [1]. Another example is in-situ FIB cutting that can be used to preserve 3D morphology better than top-down sputter profiling and even allows 3D reconstruction using a slice and view approach [2]. Performing a FIB cut in-situ is particularly interesting for sensitive samples so that the sample can be analysed directly without any modification. This is well illustrated by recent our work using a tiltable in-situ cryo holder and argon cluster sputtering to cross-section biological samples whilst maintaining temperatures of below -140°C before performing TOF-SIMS imaging [3]. This approach is compared to results from samples that are sectioned ex-situ using cryo-microtomy and transferred and analysed under cryo conditions. Finally, the correlation of high-resolution TOF-SIMS images and SEM images from the same area will be presented alongside novel denoising algorithms to improve signal to noise ratio without sacrificing lateral resolution [4,5].
This work was carried out on the Platform for Nanocharacterisation (PFNC) of CEA-Grenoble, supported by the “Recherche Technologique de Base”, “3D-Lipid” InterCarnot Project between CEA-Leti and 3BCAR institutes and "France 2030 - ANR-22-PEEL-0014" programs of the French National Research Agency (ANR).

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Quantification of amine surface functionalisation of SiO_2 nanoparticles by ToF-SIMS in combination with XPS and qNMR

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Engineered nanoparticles (NPs) with surface functionalities are increasingly used in different applications, including medical diagnostics, catalysis, sensing, and energy technologies. To support the manufacturing industry and regulatory authorities, the SMURFnano project aims at developing robust and standardized methods for quantification of NP surface functionalities and coatings using a combination of chemical analysis techniques. In this study, ToF-SIMS was used for quantification of amine functional groups on SiO_2 NPs, where correlation with XPS and qNMR provided calibration with respect to N surface concentration and amine NP concentration, respectively. ToF-SIMS and XPS analyses of the same sample batches were conducted independently at two laboratories (RISE and JSI). Amorphous non-porous SiO_2 NPs (80 nm) were synthesized by a sol-gel process at BAM and amine modification was done in a grafting step using 3-aminopropyltriethoxysilane (APTES) [1]. For ToF-SIMS and XPS analysis, multilayer NP deposits were dropcasted onto gold-coated silicon substrates from ethanol suspensions. The results indicate linear relationships between the ToF-SIMS intensity ratio and quantitative results from qNMR and XPS (Figure 1), to suggest that ToF-SIMS can be a powerful method for quantification of amine functional groups on SiO_2 NPs, after calibration.

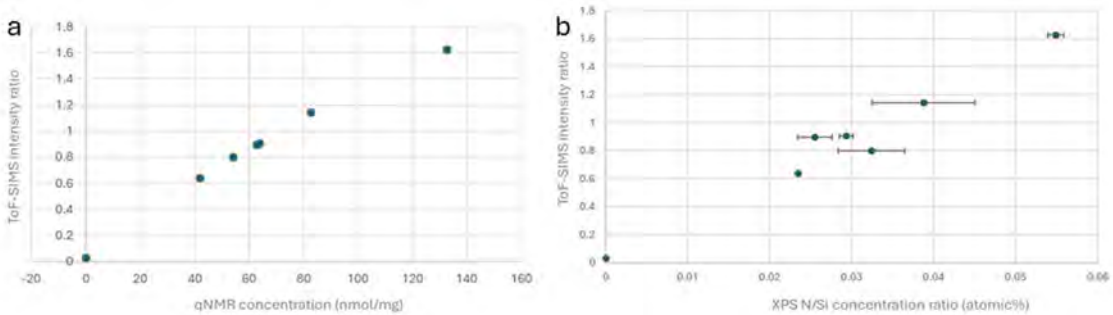


Figure 1 Correlation between ToF-SIMS intensity ratios (peaks representing amine/silica) and (a) amine concentration determined by qNMR, and (b) XPS atomic concentration ratio (N/Si).

The project (23NRM02 SMURFnano) has received funding from the European Partnership on Metrology, co-financed from the European Union's Horizon Europe Research and Innovation Programme and by the Participating States.

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Nickel Electrode Degradation Pathways Probed by NanoSIMS Deuterium/^{18}O Isotopic Depth Profiling and In-Situ NAP-XPS

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Most hydrogen produced today is derived from fossil fuels such as natural gas, coal, and oil. However, growing demand for sustainable, low-carbon energy sources has driven increased interest in green hydrogen production.

Electrolysis, a process that uses electricity to split water molecules into hydrogen and oxygen [1], is the key method for producing hydrogen from renewable energy. When powered by solar, wind, or other renewable sources, electrolysis provides a clean and sustainable pathway to hydrogen production. Despite this potential, large scale deployment is still limited by an incomplete understanding of the catalyst surface chemistry and associated reaction mechanisms

Nickel has historically been favored as an electrode material for water electrolysis, particularly from the 1920s through the 1970s, because of its resistance to alkaline conditions, favorable electrochemical properties, and relative affordability [2]. While nickel catalysts show strong performance, they are prone to degradation over time. Research indicates that nickel electrodes lose effectiveness during prolonged usage due to the formation of nickel hydride on the electrode surface [3].

In this study Ni thin films were subjected to electrochemical degradation tests and characterised using Near Ambient Pressure X-ray Photoelectron Spectroscopy (NAP-XPS) and Nanoscale Secondary Ion Mass Spectrometry (NanoSIMS). NAP-XPS enabled investigation of the nickel catalyst under controlled water and gas environments. By developing a quasi in-situ droplet system, we also performed electrochemical tests directly within the NAP-XPS system. This allowed us to determine the chemical species present immediately after electrochemical operation.

By introducing isotopically labelled electrolyte, NanoSIMS was able to provide detailed information on the depth distribution of hydrogen and oxygen isotopes within the nickel thin films. This enabled the determination of isotope incorporation and localisation within the nickel films. Combining NanoSIMS isotopic labelling and NAP-XPS allowed us to uncover insights into the surface reactions occurring during and after electrochemical operation. These results offer valuable understanding of the operation and degradation of alkaline nickel electrolysers.

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High-Resolution Microscope-Mode Secondary Ion Mass Spectrometry Imaging

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This study presents a transformative approach to Mass Spectrometry Imaging (MSI) that takes advantage of high-speed data acquisition while further optimising the possible mass and spatial resolution and broadening the detectable mass range. MSI is a powerful analytical tool capable of identifying unknown species while providing mass-specific surface images with micron- or submicron-level spatial resolution. By transitioning from the conventional microprobe to microscope mode and incorporating Secondary Ion Mass Spectrometry (SIMS) imaging with intensified Charge-Coupled Device (CCD) and Complementary Metal-Oxide Semiconductor (CMOS) cameras, this work demonstrates substantial gains in speed, throughput and imaging qualities.

A defocused buckminsterfullerene (C_{60})-based cluster source was employed as the primary ion beam. Mass resolution was enhanced through novel ion bunching and time-dependent Post-Extraction Differential Acceleration (PEDA) techniques, underscoring the effectiveness of time-variable PEDA. The experimental results illustrate the mass resolution of $m/\Delta m$ ~2000 across a mass range of $m/z \geq$1000, and this could further improve to $m/\Delta m$ ~6900 with the application of a fast scintillator [1]. Our investigation into spatial resolution highlights the complex relationship between magnification, signal integrity, and image distortion, offering practical strategies for optimising spatial accuracy. Under optimum conditions, spatial resolution yielding better than 5 μm was achieved [1]. Additionally, the integration of time-of-flight imaging using the Timepix3 camera provides a precise solution. Ongoing development will explore next-generation detectors such as Timepix4, which are expected to offer improved timing precision and higher data throughput. SIMION 2020 is used to assist in modelling adjustments of the geometry to the ion optics and predicting corresponding experimental results to widen the detectable mass range while preserving good spatial resolution and increasing the mass resolution. Overall, this work is expected to lay the groundwork for commercial adoption in clinical diagnosis applications and further advance the capabilities of MSI.

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Glycosaminoglycan patterning in early embryonic development using ToF-SIMS

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Glycosaminoglycans (GAGs) are long, linear polysaccharides composed of repeating disaccharide units, found throughout the extracellular matrix and on the surface of virtually all cells in the body. Heterogeneity in their sulfation patterns, lengths and conformations results in extraordinary structural complexity, underpinning their wide-ranging biological functions whilst posing a significant analytical challenge. Unlike other biopolymers, GAG biosynthesis is non-template driven yet, GAGs are associated with cell-specific patterns established during early development as well as in diseases such as infection, neurodegeneration and cancer. Traditional methods of analysing GAGs are limited in their ability to only collect either spatial or compositional information. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a powerful technique offering label-free, *in situ* GAG analysis capable of providing simultaneous spatial and compositional information. GAG discriminatory ions have been validated based on their presence in the spectra of purified GAG reference samples combined with their presence or absence in wild-type and GAG biosynthetic enzyme knockout cell lines, respectively.

GAGs are implicated in a multitude of processes during early embryonic development including tissue patterning, axis formation and cell differentiation. Gastruloids are 3-dimensional embryonic stem cell-derived self-assembling aggregates that recapitulate key features of early embryonic development including symmetry breaking, axis patterning and germ layer formation. This model provides a reproducible system for studying how GAGs are organised within the developing embryo and how their spatial organisation and composition are dynamically regulated during the developmental process. Sectioned mouse and human gastruloids from multiple timepoints and developmental stages were analysed using ToF-SIMS. Correlative immunofluorescent staining for lineage marker expression was used to validate sample selection and enabled the detailed spatial mapping of GAGs in the context of additional extracellular matrix components. ToF-SIMS was able to assess spatial and compositional changes in multiple GAG types throughout gastrulation and detect differences between mouse and human lineages, demonstrating the utility of ToF-SIMS for unlabelled analysis of biomolecules within biological samples.

GCIB-Assisted Reactive Landing of Peptides and Proteins on Functionalized Surfaces

Mehdi Lakhdar, Christine Dupont-Gillain and Arnaud Delcorte

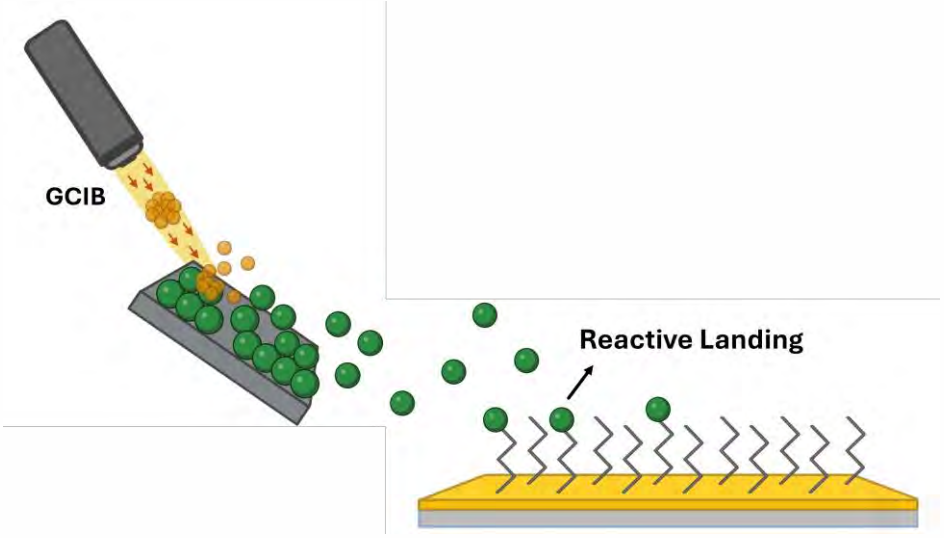
Institute of Condensed Matter and Nanosciences - UCLouvain, Louvain-la-Neuve (Belgium)

Gas cluster ion beam (GCIB)-assisted transfer is investigated as a solvent-free approach for the deposition and immobilization of biomolecules on functionalized surfaces. A model system based on the cyclic peptide Cyclo-(RGDfK) was studied on gold substrates modified with 3-mercaptopropionic acid NHS ester (3-MPA NHS) self-assembled monolayers. Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) reveals the formation of a characteristic peptide–SAM adduct under GCIB deposition, consistent with covalent immobilization. Rinsing experiments further support this interpretation through selective retention of surface-bound species.

A dose-dependent study of Cyclo-(RGDfK) transfer further allowed distinguishing different deposition regimes on the SAM, ranging from initial surface coverage to the formation of peptide multilayers at higher doses.

This approach was extended to the redox-active microperoxidase-11 (MP11). ToF-SIMS confirms successful transfer and enhanced retention on reactive SAMs compared to bare gold after rinsing. Complementary bioactivity assays performed on surface-confined enzymes indicate preservation of catalytic function. Ongoing work explores the electrochemical characterization of immobilized MP11 using cyclic voltammetry, with the aim of probing electron transfer processes at the enzyme–surface interface and further assessing the nature and functionality of the immobilization.

These results demonstrate the potential of GCIB-assisted deposition for the fabrication of functional biointerfaces beyond the limitations of conventional solution-based approaches.



ToF-SIMS examination of IgG Antibody Orientation on Multimolecular Protein- and Lipid-Based Layers on Silicon

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Biosensors rely on well-engineered recognition layers to achieve selective detection of analytes in complex samples. Immunosensors utilize immunoglobulins as biorecognition elements, taking advantage of their high specificity and selectivity towards antigens. Preserving antibody functionality upon immobilization on solid surfaces (correct orientation, lack of denaturation) is essential for sensor performance. In particular, antibody orientation on the surface (flat-on, side-on, tail-on, or head-on) determines antigen-binding efficiency by controlling access to the antigen-binding sites located on the Fab domains.

This study demonstrates the capability of Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) combined with Principal Component Analysis (PCA) to determine the orientation of goat anti-rabbit IgG antibodies (IgG) on multimolecular layers composed of proteins and lipids. Four types of silicon surface modifications were investigated: protein G (which binds specifically to the Fc region of IgG); streptavidin–biotin interaction; and Langmuir–Blodgett-deposited sphingomyelin-based monolayers. Immobilization of IgG from solutions of varying concentrations, as well as subsequent binding of rabbit IgG antigen, were monitored in real time using White Light Reflectance Spectroscopy equipped with a microfluidic cell. ToF-SIMS combined with PCA was applied to examine the surface composition of the multimolecular layers and to analyse IgG orientation based on the compositional differences between the Fc and Fab regions of antibody. A surface density dependent analysis of IgG orientation was employed to accurately determine the dominant vertical orientation of IgG. [1,2]

Surface functionalization with protein G promoted a tail-on orientation at IgG surface density forcing vertical alignment. In contrast, streptavidin-functionalized surfaces yielded predominantly side-on attachment of biotinylated IgG with a low maximal surface coverage. IgG adsorption on lipid monolayers resulted in mixed orientation with tail-on to head-on ratio of 3:1.

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OrbiSIMS imaging reveals spatial localizations of omega-3 and omega-6 fatty acids during brain development

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Omega-3 and omega-6 polyunsaturated fatty acids (PUFAs) are essential dietary nutrients required for brain development and function. Imbalance between omega-3 and omega-6 PUFAs is a feature of many western diets and there is evidence that this is likely to be detrimental for neurological health [1]. Despite this clinical importance, it is not yet understood how PUFAs vary from one brain cell type to another nor how they promote optimal neuronal function. Here we address both knowledge gaps in the context of the genetic model organism *Drosophila*, which has a brain that is well characterized at the single-cell level [2,3]. Utilizing the OrbiSIMS platform [4,5], we have developed optimized workflows for mapping the distributions of more than 200 metabolites, including PUFAs, in the brain with high spatial and mass resolution during development and adulthood. These brain atlases reveal that PUFA containing lipids show striking region-specific distributions across the brain during development. Together, our findings demonstrate that OrbiSIMS provides new biological insights into the cell-type specific regionalization of PUFAs during brain development and aging.

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Schinzel-Giedion Syndrome and RNA-therapy - Molecular effects on oligodendrocyte models revealed by ToF-SIMS

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Schinzel–Giedion syndrome (SGS) is an ultra-rare disorder caused by gain-of-function mutations in *SETBP1*, leading to protein accumulation and widespread cellular dysregulation [1]. One of the detrimental consequences of SGS is epilepsy, potentially caused by the dysregulated myelination in oligodendrocytes [2]. Antisense oligonucleotides (ASOs) offer a promising medical strategy to reduce SETBP1 levels in a targeted manner, but their effects on the molecular composition of oligodendrocyte plasma membrane remain poorly understood [3]. Here, we used ToF-SIMS imaging to investigate SGS-associated lipid dysregulation and ASO-mediated SETBP1 downregulation effects in the oligodendrocytes from an SGS mouse model and SGS patients.

ToF-SIMS revealed broad molecular alteration in the mouse oligodendrocyte's plasma membrane lipids. In negative ion mode, approximately 15% of detected m/z features were significantly altered in SGS compared to WT cells, with approximately 90% of those showing decreased abundance (e.g., FA 16:0). More than half of these SGS-associated features showed full or partial rescue following ASO treatment, meaning their intensities are recovered to the levels of those in the WT (e.g., FA 12:0). In positive ion mode, about a third of the detected features were altered by SGS, and a substantial portion of them were fully rescued after ASO treatment (e.g., PC 34:1). Comparison between SGS human and mouse oligodendrocyte models using a concordance analysis, SGS-associated lipid alterations were found to be conserved across the two species, highlighting molecular changes that may be prioritized for future translational studies (e.g., FA 20:3). In addition, species-specific and discordant features were also observed, indicating that some SGS-associated alterations are species dependent and should be interpreted with caution (e.g., FA 12:0).

ToF-SIMS imaging provides evidence that SGS disrupts the composition of oligodendrocyte membrane lipids and that ASO-mediated SETBP1 downregulation partially restores disease-associated molecular alterations. In contrast, cross-species profiling provides distinguished lipid signatures from species-specific variation.

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Development of Rapid Depth Profiling for Organic-Inorganic Multilayer Devices Using SF_6 Reactive Gas Cluster Ion Beam

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The development of next-generation energy storage and display technologies, including all-solid-state lithium batteries and organic light-emitting diodes, necessitates precise nanoscale characterization of complex buried interfaces. Conventional argon gas cluster ion beam secondary ion mass spectrometry remains a standard tool for organic depth profiling [1], yet it faces a critical bottleneck when analyzing inorganic or metallic layers due to extremely low etching rates.

This study proposes the implementation of sulfur hexafluoride (SF_6) reactive gas clusters as an alternative to overcome these limitations in multilayered device analysis. Reactive gas clusters provide a chemical sputtering component that significantly enhances the ionization and removal efficiency of inorganic materials compared to the purely physical interaction of Ar clusters [2, 3].

The experiment was performed on a Cr/Alq3/NPB (10 nm/100 nm/100 nm) multilayer structure fabricated on a silicon substrate via physical vapor deposition (PVD).

The depth profile demonstrated high-speed and uniform etching across both the organic and metallic domains without significant preferential sputtering or interface broadening. The chemical structures of the organic layers were well preserved throughout the sputtering process, as evidenced by the stable intensity of characteristic molecular ions.

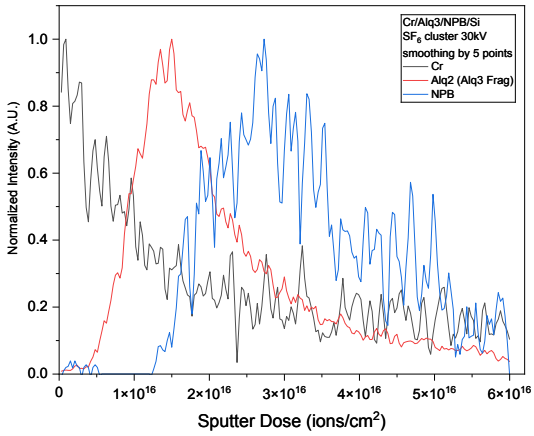


Figure 1. Depth profile of the organic-inorganic multilayer device using SF_6 gas cluster ion beam at 30 kV.

These results demonstrate that SF_6-GCIB-SIMS provides a high-speed depth profiling framework for organic-inorganic hybrid multilayer devices, overcoming the fundamental limits of conventional inert gas clusters.

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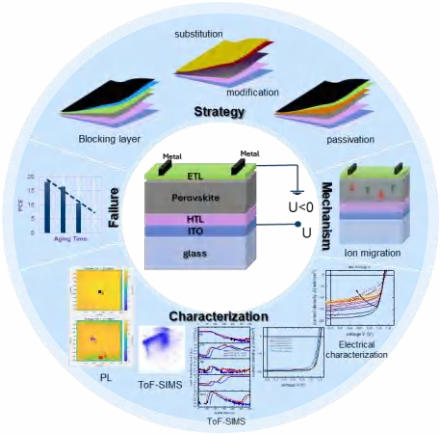
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Unravelling Ion Migration Pathways in Perovskite Solar Cells Using ToF-SIMS: Reverse bias Stability of PSCs

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Perovskite solar cells (PSCs) are among the most promising next-generation photovoltaic technologies, combining high efficiency with low manufacturing costs. However, long-term stability remains a critical barrier for commercialization. One of the primary degradation mechanisms is chemical instability and ion migration within the perovskite layer, which leads to performance losses and phase instability.

Bias-induced degradation in organo-lead halide perovskites is initiated by the generation of iodide interstitials at the interfaces between the perovskite layer and the adjacent charge transport layers. These small, mobile anions redistribute under voltage stress, altering the built-in potential of the device and migrating toward the thin Ag electrode, where they contribute to resistance changes and the formation of corrosive AgI. While trap annihilation of certain iodide defects occurs near the anode, the accumulation of negatively charged iodide interstitials near the cathode has been found to be particularly detrimental to solar cell efficiency.

This project firstly aims to investigate the impact of ion migration on the electrical and optoelectrical performance of the solar cells, comparing the different stacking of the devices by altering the transport layers and perovskite layers, while later investigating the ion migration phenomena using Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), a high-resolution technique capable of depth-profiling chemical species with sub-micron spatial precision. Our experiments are performed with the TOFSIMS5.ncs (IonTof GmbH, Muenster, Germany) in dual beam mode (30kV Bi+ for analysis; 500eV Cs+ for sputtering). Charge compensation is carried out by using the neutralizer as well as the surface potential capability of the SIMS instrument, calibrated on the most insulating perovskite layer.

In the current phase of the project, reverse-bias characterization of the solar cell stacks glass /ITO /4PADCB /$Cs_{0.05}(FA_{0.93}MA_{0.23})_{0.95}Pb(I_{0.77}Br_{0.23})_3$ /C60 /BCP /Ag and glass /ITO /4PADCB /$Cs_{0.05}(FA_{0.93}MA_{0.23})_{0.95}Pb(I_{0.77}Br_{0.23})_3$ /C60 /SnO_2 /Ag shows that devices containing the BCP layer exhibit less stable electrical behavior compared to the SnO2-based stack, likely due to the more compact and robust nature of SnO_2 relative to the softer organic BCP layer. In addition, comparison of different perovskite formulations indicates that the MA-free perovskite composition demonstrates improved stability under reverse bias conditions. Voltage-dependent photoluminescence measurements before and after reverse-bias stressing helped identify the regions of interest for ToF-SIMS depth profiling. Furthermore, ToF-SIMS analysis before and after stressing confirms electrochemically induced I^- ion migration toward the Ag electrode, leading to the formation of a local shunt path.

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Lateral Copper Diffusion in Processed VCSELs: Ion Beam Cross-Sectioning and Device-Level SIMS Analysis

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Vertical-cavity surface-emitting lasers (VCSEL) present an immense measurement challenge. These structures are composed of hundreds of layers, and their active regions consist of nanometer-scale thin layers.

A refined SIMS-based measurement procedure, which eliminates artifacts in epitaxial VCSEL structures, has been developed.[1] Building on this capability, the present work focuses on SIMS analysis performed directly on fully processed devices, where additional challenges related to complex geometry and processing-induced effects are addressed.

In reliability studies, copper contamination has been suggested as a degradation factor. Initial SIMS pad measurements, however, reveal only minor surface-level copper that does not correlate with electrical degradation. To address this discrepancy, the device is prepared in situ by ion beam cutting using two independent ion sources oriented orthogonally, enabling removal of the surrounding material and isolation of the mesa structure as a pillar-shaped feature with a square base.

Subsequent SIMS measurements, performed with a stationary primary beam aligned to avoid lateral erosion, reveal significant copper in the p-DBR and active region, with smaller amounts in the upper n-DBR layers that diminish as the pillar is sputtered down to the non-structured region of the wafer. This behavior suggests lateral copper diffusion.

Rotation of the pillar enables side-to-side SIMS analysis of the device structure. The resulting profiles reveal a pronounced U-shaped copper distribution, with significantly deeper penetration on the p-side than on the n-side, and preferential diffusion along GaAs layers compared to AlGaAs. Backtracking this behavior indicates that copper is initially deposited at the mesa sidewalls during etching, while subsequent processing, in particular aperture oxidation, activates its diffusion and drives it into the device structure.

This study demonstrates that only device-level analysis allows reliable identification of contamination sources, whereas measurements on epitaxial structures or SIMS pad regions remain insufficient to resolve the underlying mechanisms. The presented approach further establishes a pathway for SIMS analysis of materials and devices with complex three-dimensional morphology, extending its applicability beyond conventional planar structures. This capability opens new opportunities for the investigation of processing-induced effects and contamination phenomena in advanced semiconductor devices.

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Multi-dimensional Insights into the Battery Materials by ToF-SIMS

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Time-of-flight secondary ion mass spectrometry (ToF-SIMS) has emerged as a pivotal analytical technique for characterizing the complex surface and interfacial chemistry of battery materials. This review article comprehensively discusses the fundamental principles and unique attributes of ToF-SIMS, highlighting its advantages such as ultra-high surface sensitivity (ppm-ppb), high spatial resolution (<50 nm laterally, and <1 nm in depth), and high mass resolution for hydrogen and isotope study. In the field of battery study, these attributes enable precise, multi-dimensional characterization of electrode-electrolyte interphases (EEIs). In the previous works, ToF-SIMS has been employed to resolve the composition and structures at a nanoscale of EEIs, track the dynamic evolution and degradation of electrode surface, differentiate artificial coating interphases from the bulk materials and detect isotopes for mechanistic studies. The burgeoning field of *in situ* liquid ToF-SIMS for probing the authentic solvation structures and aging mechanism of electrolytes is also highlighted. Challenges of using ToF-SIMS for battery study, such as the matrix effects, beam-induced damage, and need for higher sensitivity and depth resolution are also discussed. In summary, ToF-SIMS provides multi-dimensional insights into battery interfaces, which helps to establish structure-property correlations and will continuously guide the rational design of the next-generation high-performance energy storage systems.

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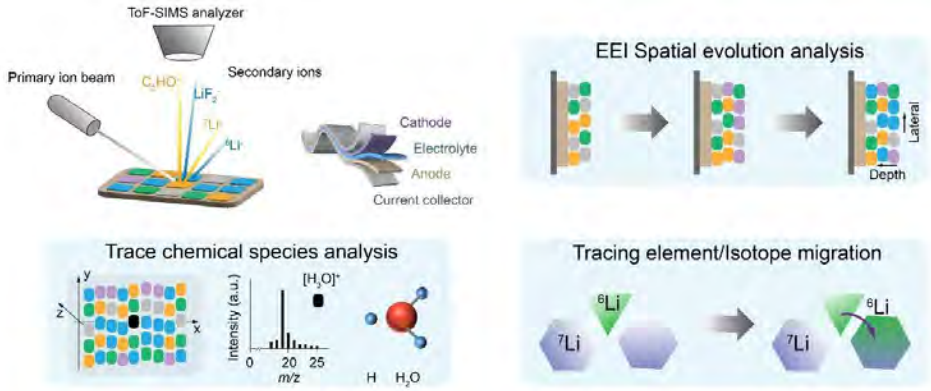


Figure 1. Schematic illustration of characteristic applications of ToF-SIMS in battery interface characterization.

In Situ Liquid ToF-SIMS Metabolomics Analysis of Single Living Cells

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Single-cell mass spectrometry enables label-free and high-throughput molecular analysis of individual cells. However, conventional vacuum-based secondary ion mass spectrometry (SIMS) faces challenges in probing metabolism of single living cells under native physiological conditions.

Here, we introduce a liquid SIMS platform coupled with a vacuum-compatible cell-culture device, which allows in situ metabolomic profiling of single living cells in their native culture environment without any pretreatment [1]. This platform uniquely enables direct nanoscale interfacial characterization, and we report for the first time the determination, via MS depth profiling, of a lipid bilayer with a SiN-equivalent thickness of ~8.6 nm in a single living human non-small cell lung cancer (A549) cell. As a proof of concept, we applied this method to investigate metabolomic changes linked to cisplatin resistance in A549 cells. Our findings indicate upregulation of cholesterol, phosphatidylcholine, and low-unsaturation fatty acids in resistant cells, and demonstrate that inhibiting cholesterol synthesis effectively reduces drug resistance. This work underscores the potential of liquid SIMS for in situ metabolic profiling during complex biological processes.

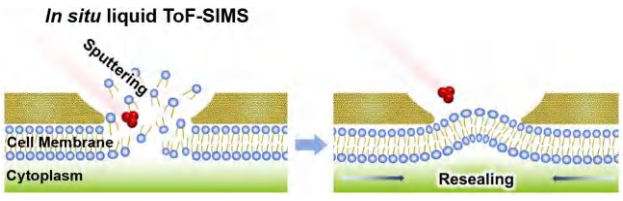


Figure 1. Schematic of in situ liquid SIMS analysis of a single living cell, gaining from the resealing of plasma membrane.

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New insights into developing brain metabolism with multiomics

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Early development is a critical window in the lifetime of an organism that shapes its future health prospects during adulthood and ageing. Extensive work in the field of the Developmental Origins of Health and Disease (DOHaD) has demonstrated that environmental stresses such as poor nutrition during early life can significantly increase the risk of a wide range of health conditions in middle- and old-age including heart disease, stroke and type 2 diabetes[1]. Many of these pathological outcomes are thought to involve dysregulated metabolism but conventional mass spectrometry often lacks sufficient spatial resolution to map this to the cell type(s) that are the main disease focus. This unmet clinical need has been addressed via the development of OrbiSIMS mass spectrometry imaging[2] and a cryogenic analytical platform for this technique[3,4]. Switching from an argon to a CO_2 primary ion beam is known to improve lateral resolution on ToF-SIMS instruments by more than 2-fold[5] and here we implement this advancement for OrbiSIMS. Using the well characterized brain of the genetic model organism *Drosophila* as a proof-of-principle, we show how OrbiSIMS imaging datasets can be combined with single-cell RNA sequencing to provide correlative metabolomics and transcriptomics atlases. This multiomics approach provides new insights into the impacts of early-life environmental stresses on brain metabolism and gene expression that may be relevant for understanding DOHaD.

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Integrated TOF-SIMS/MALDI-TOF Platform for Multimodal Molecular Imaging of Mouse Cerebellum.

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Mass spectrometry imaging (MSI) allows the spatially resolved analysis of molecular species directly in biological tissues while preserving their structure. Unlike bulk analytical techniques that require tissue homogenization or labeling-based histological methods, MSI enables direct, spatially resolved detection of a wide range of molecules such as lipids, proteins and metabolites within intact tissues.

Among MSI techniques, time-of-flight secondary ion mass spectrometry (TOF-SIMS) and matrix-assisted laser desorption/ionization time-of-flight (MALDI-TOF) are complementary. TOF-SIMS provides high spatial resolution up to 50 nm and is well suited for detecting small molecules, whereas MALDI-TOF enables the analysis of larger biomolecules such as peptides and proteins.

In this study, both techniques were applied to a mouse cerebellum tissue section. TOF-SIMS (PHI nanoTOF 3^+, ULVAC-PHI), revealed the distribution of low-mass species and fine structural features such as phosphocholine (Fig. 1b), while MALDI-TOF (iMScope™ QT, Shimadzu) provided information on higher molecular weight compounds linked to specific cell types like sulfatides. By combining and overlaying the datasets, a more complete molecular picture was obtained (Fig. 1a), improving the distinction between different cellular populations. This approach highlights the advantage of multimodal MSI for a more comprehensive characterization of biological tissues.

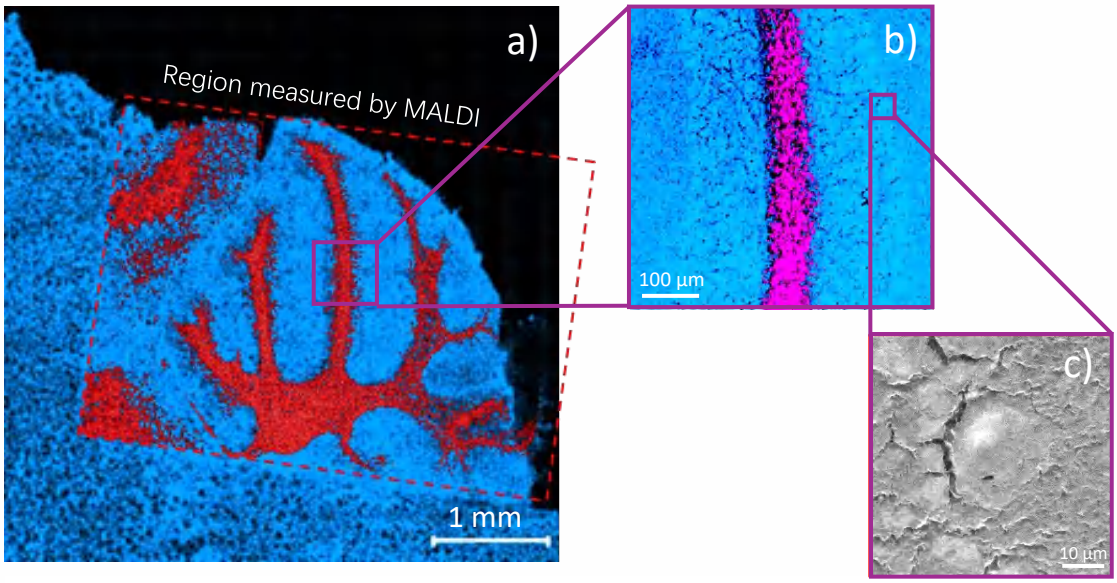


Figure 1. a) Overimposition of TOF-SIMS and MALDI-TOF imaging. Blue is phosphocoline (TOF-SIMS) and red is sulfatide (MALDI-TOF). b) Detail of TOF-SIMS imaging of cerebellum portion (500 µm FOV). Blue is phosphocoline, purple is cholesterol. c) Detail of TOF-SIMS imaging of cerebellum portion (50 µm FOV) where it is possible to distinguish single cells.

Quantitative Cryogenic Orbitrap Secondary Ion Mass Spectrometry: Characterisation of Lipid Nanoparticles

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Lipid nanoparticles (LNPs) have shown therapeutic utility as delivery vehicles for RNA, however, the way in which LNP chemical composition affects functional mRNA delivery is not completely understood. Stratified molecular analysis of LNPs can provide improved structure-function relationship information relevant to potency and tissue tropism in vivo, but the techniques available to achieve the required interfacial characterization are limited. SIMS has shown great potential for stratifying the lipid component of LNPs, with a prior study using qualitative depth profiles to confirm the basic structural arrangement of polyethylene glycol (PEG) lipids and RNA.[1] This is the first report of the application of Quantitative cryogenic orbitrap secondary ion mass spectrometry (Q-Cryo-OrbiSIMS) to model four lipid components of LNPs, using quantified ion intensity profiles to plot the composition with depth. Combinatorial spot-in-spot mixing of the four lipid components was used to generate 337 spots as a micro array on a glass slide. OrbiSIMS data was acquired from each spot. A variety of data pre-processing approaches were compared to scale the secondary ion intensity to minimise the effects of noise bias before construction of a calibration model. An artificial neural network model was used to predict the four lipid compositions from the ion intensities produces a mean absolute error (MAE) of 14 %. The model was then used to predict quantitative molecular distributions from the OrbiSIMS profiles of cryogenically preserved LNPs demonstrating the feasibility of Q-Cryo-OrbiSIMS for LNPs, as well as the potential of this method for wider application to organic systems when suitable calibrant samples are available.

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A combined OrbiSIMS and LC–MS/MS workflow reveals metabolomic and proteomic alterations in ApoE4-expressing H4 neuroglioma cells

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Apolipoprotein E (ApoE) is primarily released by astrocytes in the brain, where it binds lipids to form lipoprotein complexes that interact with soluble amyloid-β (Aβ) released from neurons. These complexes subsequently bind to receptors on microglia, astrocytes, and the blood–brain barrier to activate Aβ clearance pathways. However, individuals carrying the ApoE4 allele have a 3–12-fold increased risk of developing Alzheimer's disease (AD) compared with non-E4 carriers. ApoE4 is therefore considered one of the most significant genetic risk factors associated with AD pathology, including amyloid-β deposition, tau phosphorylation, and neuroinflammation.

Due to the complex and cell-type-specific roles of ApoE4, multi-omics approaches are widely used to identify disease-related molecular alterations. Conventional workflows typically involve tissue dissociation, cell sorting, and separate extraction steps for different chemistries, followed by LC–MS/MS analysis for metabolomics, lipidomics, and proteomics. However, these methods often require lengthy sample preparation and may lead to metabolite loss or degradation during processing. To address these limitations, we propose Orbitrap secondary ion mass spectrometry (OrbiSIMS) as an untargeted screening tool to investigate ApoE4-associated molecular changes in brain cells. OrbiSIMS enables *in situ*, label-free analysis with minimal sample preparation and has been applied on single cell metabolomics study [1].

In this study, we present a workflow using OrbiSIMS depth profiling as a rapid screening approach to characterise metabolic alterations in ApoE4-expressing neuroglioma (H4) cells [2]. The subsequent LC-MS/MS method was selected based on the OrbiSIMS results for further polar metabolomics and proteomics analyses to investigate broader ApoE4-associated molecular and protein changes. The combined workflow revealed disruptions in lipid metabolism, particularly in glycerophospholipid and sphingolipid pathways, as well as in amino acid metabolism. Proteomic analysis further confirmed alterations in amino acid metabolism and tRNA aminoacylation processes and identified changes in RNA splicing pathways. Overall, this study demonstrates that OrbiSIMS provides a rapid, extraction-free, untargeted metabolomics screening strategy for investigating ApoE4-associated molecular alterations and has strong potential for application to more complex brain cell co-culture systems to study intercellular interactions.

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Exploring SIMS-Related Phenomena through Recent Computer Simulations

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Cluster ion beams provide unique opportunities for the analysis of molecular and low-dimensional materials. However, the microscopic mechanisms of energy deposition, sputtering, and molecular emission strongly depend on the properties of both the projectile and the target. Molecular dynamics (MD) simulations provide direct insight into these ultrafast processes at the atomic scale.

In this presentation, we will discuss recent MD studies of cluster-induced sputtering, with particular emphasis on water cluster projectiles. Topics will include the formation and ionization of water clusters, the bombardment of water and ice at different temperatures, and the interaction of 20 keV water cluster projectiles with trehalose, including systems covered by a thin ice layer. The influence of projectile temperature and internal degrees of freedom on energy deposition and sputtering, as well as the effects induced by very large water clusters, will also be addressed.

An important part of the discussion will focus on the differences between sputtering of bulk materials and monolayer systems. The latter will be illustrated by C_{60} bombardment of free-standing graphene and graphene supported on a silicon substrate, demonstrating how the presence of an underlying substrate can significantly modify energy dissipation, damage formation, and material ejection.

These examples illustrate how atomistic simulations can help identify the key parameters governing cluster-induced sputtering and provide a microscopic interpretation of phenomena relevant to SIMS analysis.

Predicting polymer mass spectra via molecular dynamics simulations

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Polymers constitute a versatile class of materials whose applications include high-performance electrolytes in next-generation batteries, critical insulating layers in microelectronics, medical devices, and global packaging logistics. However, the chemical stability that makes polymers durable also renders them persistent environmental pollutants (microplastics) which can contaminate food chains. Accurate chemical characterization is therefore required to optimize their industrial manufacturing and evaluate their environmental impact.

Mass spectrometry is widely recognized as a technique of choice for detecting and identifying polymers. Secondary ion mass spectrometry (SIMS) is particularly interesting due to its high surface sensitivity and its potential for nanoscale spatial resolution [1, 2]. However, the ion sources needed to achieve that resolution (e.g. neon) also induce extensive polymer fragmentation, an effect only exacerbated at high ion doses (above 10^{12} ions/cm^2) [3]. This fragmentation process remains poorly understood and leads to difficulty in interpreting SIMS spectra.

To address this challenge, we developed a computational workflow to simulate the SIMS process and predict the resulting mass spectra of polymers via molecular dynamics simulations. A simulated polyethylene sample of dimensions $15 \times 15 \times 15$ nm^3 is probed by a 10 keV focused Ne ion beam and studied under a range of ion doses. Employing the ReaxFF potential for C/H/O systems, we model the necessary chemical reactions to induce the formation of clusters [4].

With this contribution, we provide a theoretical baseline against which experimental spectra can be matched, and which is, in principle, applicable to arbitrary polymers. On-going work aims to extend the approach to other ion species and beam energies, as well as the addition of a water layer to account for moisture deposition.

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Comparative evaluation of molecular damage by Ar gas cluster and Bi cluster using OrbiSIMS measurements of a monodisperse polymer

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In secondary ion mass spectrometry, the low secondary molecular ion yield in the high-mass range [1] remains a limiting factor for high-sensitivity SIMS analysis. However, it is still unclear whether this arises from molecular damage or from low ionization efficiency. Therefore, this study aims to elucidate the mechanism of molecular damage using a monodisperse polymer, which provides fragment information over a wide molecular weight range. The difference in molecular damage between Ar gas cluster and Bi cluster irradiation was investigated using this sample. Measurements of the monodisperse polymer were performed using OrbiSIMS with high mass resolution, enabling more accurate analysis of fragment ions.

The sample was prepared using a mixture of a solution of monodisperse (n=45) polyethylene glycol monomethyl ether (mPEG) and a solution of sodium trifluoroacetate (Na-TFA), which was used as a cationization agent, at a volume ratio of 1:10. SIMS measurements were performed using an OrbiSIMS instrument (IONTOF GmbH).

Figure 1 shows the molecular weight distributions of singly-charged mPEG ions obtained using 20 kV Ar_{1300}^+ and Bi_3^+ irradiation. The distributions were constructed by extracting peak intensities corresponding to each degree of polymerization (n) from mass spectra obtained from SIMS measurements. The intensity (vertical axis) was normalized to the same ion dose. As shown in Fig. 1, the intensity in the molecular weight distribution obtained by Ar gas cluster irradiation remained relatively constant over the molecular weight range of 400–1800. In contrast, the intensity in the molecular weight distribution obtained by Bi cluster irradiation decreased with increasing molecular weight. Based on the assumption that bond cleavage occurs with equal probability at any bond within a molecule and produces an equal number of fragments at each degree of polymerization, it was found that, under the present irradiation conditions, Ar gas cluster irradiation induces approximately one bond cleavage per molecule, whereas Bi cluster irradiation induces multiple bond cleavages.

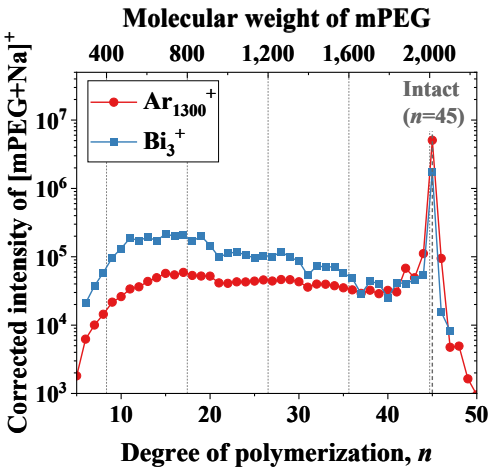


Figure 1. Comparison of molecular weight distributions of singly-charged mPEG ions by Ar gas cluster and Bi cluster irradiation.

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SIMS and Hydrogen Atmosphere: Depth Profiling, Quantitative Analysis, and Cluster Secondary Ion Formation

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Hydrogen flooding during SIMS depth profiling provides a simple, novel approach for improved analysis of multilayers and thin films composed of metals, alloys, and metal oxides. Metal hydride cluster secondary ions form selectively and specifically during depth profiling of unoxidized metals and show improved ionization of negative secondary ions [1]. This effect enables more accurate layer identification and interface determination [1]. Compared to the UHV environment, reduced surface roughening was also observed under H_2 atmosphere, enhancing depth resolution [1,2]. Furthermore, quantitative depth profiling of alloys in a hydrogen atmosphere demonstrates reduced analytical error, with improvements most evident for the transition metals. The deviations from the true atomic ratios of Ti, Cr, Fe, Co, and Ni in different alloys remained below 46% when analyzed in the H_2 atmosphere [3]. In contrast, these values reached 66% and 228% for the O_2 atmosphere and UHV environment, respectively [3].

It is evident that adsorption of hydrogen to the freshly sputtered surface reduces the substrate-induced matrix effect and creates a new, H_2-induced matrix effect that remains constant across samples, unlike the substrate-induced one. However, it was necessary to demonstrate that gas adsorption competes with ion sputtering on a relevant time scale to support this explanation. Underlying mechanisms were, to some extent, described and studied through molecular hydrogen dissociation. Atomic hydrogen was generated by introducing gas into the analytical chamber via a heated metallic capillary at 2200 K, with a dissociation yield of H_2 reaching 30% [4]. Formation of H atoms resulted in higher intensities of metal hydride cluster ions compared to their intensities measured in purely molecular H_2 [4]. A comparison of the time scales of possible processes provided insight into the mechanism of hydride cluster secondary ion formation. Cluster ions presumably form during the recombination of atoms and molecules from the sample and those adsorbed from the gas [4]. Further studies of the formation mechanism of hydride cluster ions are planned via manipulation of ion-sputtering and gas-flooding parameters.

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Chemical Imaging of Subcellular Organization and Dynamics

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Understanding how chemical composition is organized and dynamically regulated within cells is central to modern cell biology and neuroscience. Chemical imaging approaches now enable direct visualization and quantification of metabolites, lipids, and signaling molecules at subcellular resolution. One of these is mass spectrometry imaging with SIMS. Mass spectrometry imaging (MSI) has emerged as a powerful platform for mapping the chemical organization and dynamics of cells with high molecular specificity and spatial resolution. In this talk, I will highlight recent advances in development and application of techniques such as imaging mass spectrometry, nanoscale secondary ion mass spectrometry (NanoSIMS), super-resolution fluorescence microscopy, and correlative electron microscopy to subcellular imaging. Together, these methods provide complementary insights into the spatial distribution and temporal evolution of organelles, vesicles, and protein assemblies. Emphasis will be placed on integrating structural and chemical information to resolve heterogeneity within subcellular compartments, including vesicle dense core and halo regions, stress granules, and mitochondria/vesicle interfaces. Emerging strategies combining live-cell electrochemical measurements with high-resolution imaging further enable functional interrogation of processes such as exocytosis and metabolic regulation with comparison to MSI data. These developments are transforming our ability to link molecular composition with cellular function, offering new opportunities to elucidate mechanisms underlying neurotransmission, disease pathology, and cellular adaptation.

Key words : Mass spectrometry imaging, complementary imaging methods, cells, organelles, protein condensates

Advancing Nanoscale Analytics: Compact Magnetic Sector Spectrometer and Continuous Focal Plane Detector for Hyperspectral SIMS Imaging

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The constant drive toward miniaturization in materials science, coupled with the need to resolve complex interfaces in environmental and energy systems, demands analytical tools that bridge the gap between nanometric spatial resolution and high chemical sensitivity. While Focused Ion Beam (FIB) platforms are traditionally recognized for microscopy and sample preparation, recent breakthroughs in ion source technology, most notably the Low-Temperature Ion Source (LoTIS) delivering high-brightness Cs^+ beams (10^7.Acm^{-2}sr^{-1}), have paved the way for SIMS integrated in FIB platform. This contribution highlights the major technological developments led by us to transform FIB(-SEM) instruments into advanced analytical workstations, centered on a custom compact magnetic sector mass spectrometer enabling elemental and isotopic mapping with a lateral resolution reaching 15 nm.

A second, and perhaps even more transformative, technological leap is the development of a continuous Focal Plane Detector (FPD). Unlike conventional magnetic sector instruments limited to monitoring a few pre-selected ions via discrete detectors, the FPD utilizes a long microchannel plate coupled with a delay-line readout system. This setup enables simultaneous detection of the full mass spectrum (up to 500 amu) at every pixel. This hyperspectral capability brings the "post-acquisition" flexibility available in Time-of-Flight SIMS to the superior dynamic range and signal-to-noise performance of magnetic sector SIMS [1, 2].

Beyond detection, the integration of this SIMS architecture within a FIB-SEM platform unlocks a broad set of complementary capabilities that extend the analytical scope of SIMS. High-precision micromachining enables immediate in situ analysis of cross-sections or lamellas without air exposure, while specialized cryo or electrochemical modules allow studies under specific operational conditions. By correlating SIMS with EBSD, BSE, and EDX signals routinely available on the platform, these instruments provide a unique multimodal environment for holistic material characterization [1].

The analytical power of this instrumentation is demonstrated across a broad range of applications: mapping of light elements (Li, H) for degradation studies in next-generation batteries and hydrogen embrittlement; high-resolution 3D chemical profiling of complex microelectronic architectures (FinFETs, stacked nanosheets) for dopant and interfacial diffusion monitoring [1-3]. Finally, we address the challenge of managing large-scale hyperspectral datasets and the statistical workflows required to extract meaningful insights from this new generation of nanoscale SIMS data, redefining the boundaries of chemical imaging.

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High-energy-per-molecule O_2-GCIB sputtering approach for reliable molecular depth profiling of organic-inorganic hybrid nanomaterials

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Hybrid nanomaterials, composed of organic and inorganic nanometer-sized domains, have gained increasing attention for their ability to exhibit emergent properties surpassing those of their individual building blocks. To exploit these characteristics, researchers have implemented this novel class of materials in several fields, ranging from microelectronics to energy harvesting. Given their widespread application, it has become essential to develop characterization techniques capable of providing detailed chemical and structural insights into such complex systems. Although Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) has been extensively utilized for the characterization of complex samples, the disparate conditions required for the sputtering of stiff inorganic versus soft organic materials within the same matrix render the analysis of hybrid nanomaterials an ongoing challenge. The unresolved issues are primarily associated with the sputtering yield mismatch between organic and inorganic moieties when subjected to the same primary beam. Furthermore, the preservation of molecular integrity within the organic phase is frequently compromised by the overly energetic sputtering conditions necessitated by the inorganic components. To overcome these limitations, this work presents a novel approach for dual-beam depth profiling of hybrid nanomaterials consisting of high-energy-per-molecule O_2-GCIB sources as the sputtering beam. While the increased energy per impinging molecule (40 eV/m) compared to standard cluster SIMS conditions ensures an enhanced sputtering yield for inorganic components, the proposed radical scavenging ability of reactive oxygen molecules facilitates the quenching of transient active species, such as radicals, generated during the sputtering of the organic counterpart. This process prevents cross-linking and the subsequent loss of molecular information, a common limitation observed when depth profiling with alternative sources, such as argon clusters. The application of this approach to MoO_3 and arylamine NPD blends enabled the simultaneous erosion of both moieties, with sputtering yield of 20 nm^3/PI for MoO_3 and 85 nm^3/PI for NPD. Crucially, this was achieved while preserving molecular information from the organic material throughout the entire depth. This represents the first successful acquisition of reliable molecular depth profiles for such systems, effectively balancing disparate sputtering requirements [1]. By addressing these longstanding challenges, the proposed methodology provides a robust means to characterize complex hybrid architectures of technological interest, such as Organic Photovoltaic cells (OPVs).

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Challenges and Capabilities of Dual-Beam Depth Profiling at Low Sputter Energies

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In the early 1980s, Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) was developed to provide detailed elemental and molecular surface information under static conditions [1]. Over the decades, continuous technical advancements have transformed TOF-SIMS from a specialized surface spectrometry tool into an extremely flexible and versatile technique. Today, it offers not only high mass resolution spectrometry but also high-resolution imaging in the sub-100 nm range, as well as depth profiling of both inorganic and organic materials.

Depth profiling is typically performed in the so-called dual beam mode [2]. In this mode a short pulsed analysis beam generates the secondary ions, while a separate sputter beam erodes the surface during the intervening cycles to access deeper layers. The primary advantage of this approach is the parallel detection of all masses of a given polarity. This makes the technique ideally suited for screening unknown samples or for applications requiring the simultaneous analysis of numerous elements.

Although TOF-SIMS dual-beam depth profiling is the standard in both industry and academia, it presents certain limitations compared to classical single-beam depth profiling:

- **Sensitivity Constraints:** Since data is generated by a short primary pulse, sensitivity can be limited when high sputter beam energies are applied.
- **Depth Resolution Limits:** Conversely, the high energy of the analysis beam can limit depth resolution, particularly when low sputter beam energies are required.

In this contribution, we discuss the capabilities and limitations of dual-beam depth profiling at sputter beam energies ≤ 250 eV, focusing specifically on the achievable depth resolution and the resulting sensitivity.

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Approaches to the Stability of High-Level radioactive Waste glass under coupled environments and the role of ToF-SIMS

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China will organize its 11th China Secondary Ion Mass Spectrometry Conference in Nanjing in 2027. The application of ToF-SIMS in nuclear science is attracting growing interest. Our research focuses on ensuring the long-term stability of vitrified high-level radioactive waste (HLW). Experimental approaches employ coupled or sequential exposure regimens, as demonstrated in studies of ternary sodium borosilicate (NBS) and quaternary lithium borosilicate (QBG) model glasses. Key findings reveal that γ-irradiation (e.g., doses of 300 kGy to 3 MGy) induces solution acidification and promotes glass network depolymerization, evidenced by a reduction in Q^3 species and an increase in non-bridging oxygen. These changes accelerate initial ion-exchange reactions, leading to enhanced release of mobile elements like Na and B—with increases up to 30% observed. Under high-dose irradiation (e.g., 800 kGy), elemental redistribution occurs, involving surface precipitation of Na-rich particles and inward diffusion of hydrogen. However, the long-term degradation is ultimately dominated by the aqueous corrosion process itself, which forms a protective, silica-rich gel layer. Consequently, while irradiation temporarily enhances initial corrosion rates, the residual leaching rates of irradiated and non-irradiated samples converge over extended periods (e.g., after 16 days), indicating a limited long-term impact on the fundamental corrosion mechanism. Central to elucidating these complex interactions is Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). Its exceptional sensitivity for light elements and superior depth-profiling capability are indispensable for directly mapping nanoscale elemental behaviors, such as irradiation-induced Na depletion and H ingress, and for characterizing the evolving alteration layers, thereby providing critical insights into the stability of nuclear waste forms under coupled extreme conditions.

Key words: ToF-SIMS; borosilicate glass; elemental behavior; irradiation

ToF-SIMS Reveals How a CuAg Nanoparticle Hydrosol Inhibits Microbial Corrosion

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Sulfate-reducing bacteria (SRB) colonize metal surfaces and generate corrosive sulfides during metabolism, threatening critical infrastructure in sulfur-rich environments. A stable CuAg bimetallic nanoparticle (BNP) hydrosol was prepared by anchoring hydrophilic polymer chains to the particle surface, endowing it with strong antibacterial activity. ToF-SIMS depth profiling and 3D imaging were employed to compare corrosion products on steel coupons with and without BNP hydrosol treatment. Untreated coupons displayed significant sulfur and iron sulfide signals, whereas treated surfaces showed markedly reduced concentrations of these corrosive species. Notably, very little amounts of CuS or Ag_2S were detected on BNP hydrosol-exposed coupons, indicating that released Cu^+ and Ag^+ ions barely react with biogenic H_2S. These findings demonstrate that the CuAg BNP hydrosol functions simultaneously as a souring suppressant, curtailing sulfide accumulation while preserving active metal ions for sustained antimicrobial efficacy. This two action mechanism enhances both corrosion resistance and sustained antibacterial activity by suppressing the sulfide-mediated scavenging of active antimicrobial ions. The study further highlights the power of ToF-SIMS for resolving complex chemical interactions within the SRB biofilms on metallic substrates.

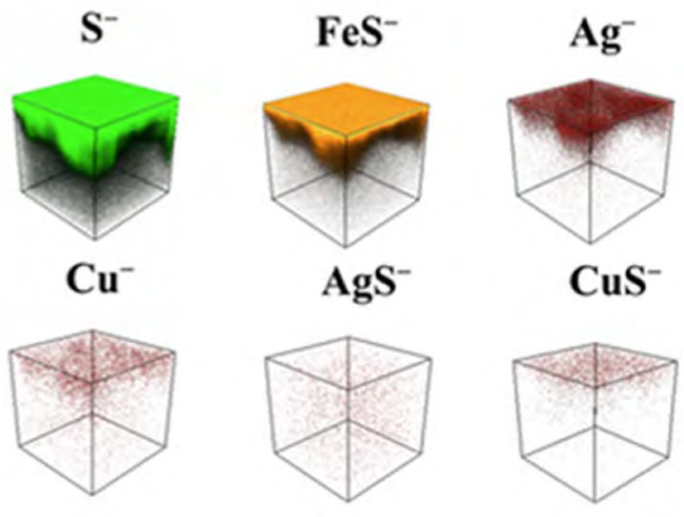


Figure 1. 3D ToF-SIMS images of the produces species after treatment with Cu-Ag BNP hydrosol

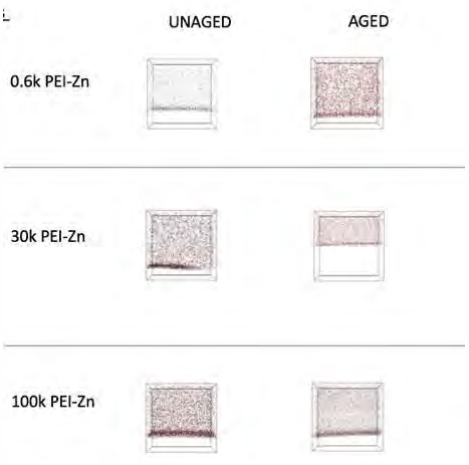
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3D ToF-SIMS Investigation of Molecular-Weight-Dependent Stability in PEI-Zn Electron Transport Layers for Organic Photovoltaics

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The long-term stability of polymeric interlayers remains a critical challenge for organic photovoltaic devices operating under harsh environmental conditions. In this work, time-of-flight secondary ion mass spectrometry (ToF-SIMS) was employed to investigate the degradation behavior of PEI-Zn electron transport layers (ETLs) with molecular weights ranging from 0.6 kDa to 100 kDa. Samples were analyzed before and after accelerated aging at 85 °C and 85% relative humidity for 200 h. Depth profiling and three-dimensional chemical reconstructions were used to characterize the distribution of characteristic ions associated with the active layer, ETL, and substrate. While all aged samples exhibited evidence of interfacial redistribution, 3D $C60^-$ mapping provided direct visualization of molecular segregation and diffusion phenomena occurring across the multilayer architecture. In particular, Zn-related signals were observed to broaden toward the active-layer interface after aging, indicating migration processes within the ETL region. The three-dimensional analysis revealed clear differences among the investigated molecular weights. High-molecular-weight PEI-Zn samples preserved a more defined layer structure and exhibited reduced chemical redistribution compared with lower-molecular-weight analogues. These observations provide direct spatial evidence that increasing polymer molecular weight enhances the resistance of the ETL to thermohygrometric stress. The results demonstrate the unique capability of ToF-SIMS 3D imaging to visualize buried-interface degradation processes and establish a direct correlation between polymer molecular weight and interfacial stability. This approach provides valuable mechanistic insight for the design of more durable electron transport layers in next-generation organic electronic devices.



Studies and Applications of SIMS in Failure Analysis of Gate Oxide Integrity in Wafer Fabrication

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As semiconductor device dimensions continue to shrink, failure analysis of gate oxide integrity (GOI) issues, such as leakage and breakdown, has become increasingly challenging. Conventional analytical techniques, including SEM, EDS, and AES, often lack the sensitivity required to detect the ultra-trace contaminants responsible for these failures. This study introduces an advanced, integrated analytical workflow that combines dynamic secondary ion mass spectrometry (D-SIMS) and time-of-flight secondary ion mass spectrometry (TOF-SIMS) to overcome these limitations. The methodology begins with electrical fault localization and chemical defect mode identification using Wright etch to differentiate between plasma-induced damage and contamination-related failures. Subsequently, TOF-SIMS is employed for comprehensive, non-targeted contamination screening, guiding precise quantitative analysis by D-SIMS (Fig.1). Two tailored analysis flows are proposed: one utilizing TOF-SIMS for contamination survey when the source is unknown, and another employing ICP-MS when a specific tool is suspected (Fig.2). Case studies demonstrate the successful identification of contaminants such as iron and molybdenum at concentrations of ~4E18 at/cm³, with root causes traced to specific fabrication line components. This workflow significantly enhances analytical efficiency, success rate, and cost-effectiveness in GOI failure analysis in wafer fabrication.

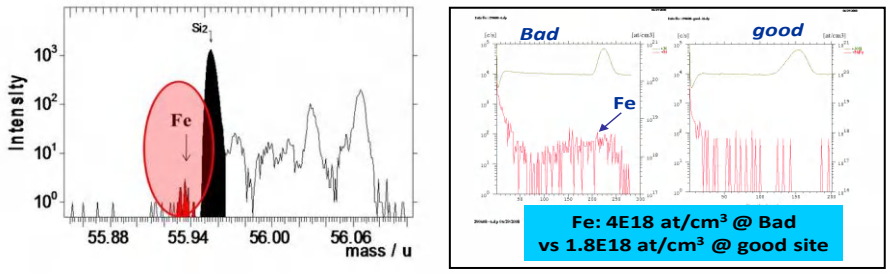


Fig.1. TOF-SIMS survey found Fe contamination on the failed sample (left). D-SIMS detected Fe contamination on the bad sample (right).

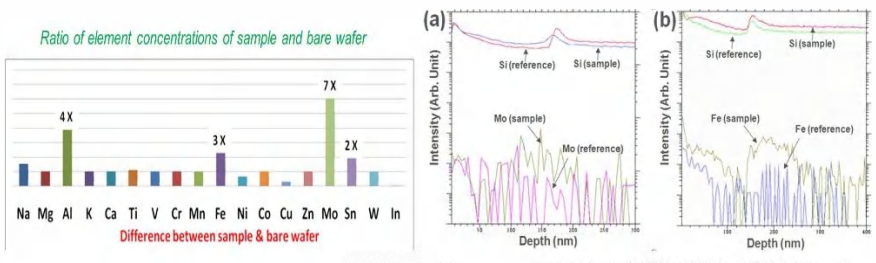


Fig.2. ICP-MS analysis was used for investigation and results showed abnormalities in aluminum (Al), iron (Fe), molybdenum (Mo), and tin (Sn) elements (left). D-SIMS quantitative analysis confirmed that the content of molybdenum and iron in the failed sample was higher than those in the normal sample (right).

Operando SIMS to Monitor Degradation in Solid-State Batteries

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The cathode electrolyte interphase (CEI) is a key determinant of the performance and long-term stability of solid-state batteries (SSBs). Forming at the interface between the cathode active material (CAM) and the solid electrolyte (SE), the CEI contributes substantially to impedance growth and capacity fading during cycling. Nevertheless, its dynamic evolution, chemical composition, and potential redox activity as a function of the state of charge (SoC) remain poorly understood, particularly in argyrodite-based systems. In this work, a novel operando ToF-SIMS sample holder was developed that enables real-time electrochemical characterisation of SSBs directly within the SIMS instrument under applied pressure. This configuration permits the simultaneous acquisition of electrochemical data and surface-sensitive mass spectrometric information throughout charge and discharge. The model system comprised $LiNi_{0.82}Co_{0.11}Mn_{0.07}O_2$ (NCM) as the CAM, Li_6PS_5Cl (LPSCl) as the solid electrolyte, and In|$(InLi)_x$ as the anode.

SoC-dependent changes in the ToF-SIMS mass spectra were monitored across the first charge–discharge cycles. Key CEI-related secondary ion fragments — including PO_3^-, SO_3^-, PS_2^-, and NiO_2^- — exhibited reversible intensity variations closely correlated with the applied cathode potential, while displaying a continuous overall increase upon cycling. The systematic growth of phosphate and sulphate fragments during charging and their subsequent attenuation during discharging strongly indicate that the CEI in LPSCl-based SSBs is partially redox-active within the relevant electrochemical potential window. Two principal decomposition pathways were identified: electrochemical oxidation of the solid electrolyte, yielding Li_3PS_4, elemental sulphur, and LiCl, and CAM-involved oxidation producing transition metal phosphates, sulphates, and chlorides. Complementary electrochemical impedance spectroscopy (EIS) was employed to quantify CEI growth kinetics as a function of SoC. Invoking the Wagner diffusion model and plotting impedance magnitude of the interfacial contribution against $\sqrt{t}$, the CEI growth rate constant k was extracted, revealing a pronounced dependence on applied potential in the range of 3.5–3.9 V vs. In|$(InLi)_x$. Operando XPS measurements performed in parallel showed no discernible compositional changes, an outcome attributed to the inherently lower surface sensitivity of this technique under the conditions employed.

Collectively, these findings substantiate the hypothesis that the CEI in argyrodite-based SSBs is electrochemically active and undergoes partially reversible compositional changes during cycling. Future work will aim to deconvolute overlapping decomposition processes and elucidate their individual kinetic contributions, advancing the mechanistic understanding of CEI formation in solid-state battery systems.

Molecular Identification and Quantitative Analysis of Asian Lacquer Films Using ToF-SIMS

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Korea Institute of Science and Technology

Traditional lacquers have been used for thousands of years as surface coating materials to decorate and protect various materials such as wood, leather, cloth, paper, ceramics, and metal. Lacquers have also been widely employed as binding mediums to attach different parts of complex or artistic objects together. They can maintain highly valued properties, including beauty, gloss, and durability for a long period of time. The saps from Asian lacquer trees are composed of substituted catechol derivatives (60-70%) plant gum, glycoproteins, enzyme laccase, and water [1].
This paper provides molecular identification of several lipid species of vegetal-source Asian lacquers for application in the field of cultural heritage. ToF-SIMS were used to analyze Korean, Chinese, Japanese, Vietnamese and Myanmarese lacquers; avoiding time-consuming and destructive extraction processes. These ToF-SIMS results provided the molecular identification of a series of substituted catechols [2]. The ToF-SIMS spectra of T. vernicifluum (Korea, China and Japan), T. succedaneum (Vietnam), and Gluta usitata (Myanmar) indicated a series of urushiol, laccol, and thitsiol repeat units, respectively.
We also evaluated the compositions of mixed lacquers, and blends of the two, using ToF–SIMS and compared with the results of Py–GC/MS and HPLC. ToF–SIMS provided quantitative results for blended lacquers; provided structural information on polymeric lacquer films; and indicated the presence of dimers and trimers of mixed catechol derivatives. 3-tridecyl-1,2-benzenediol was used as an internal standard to improve the quantitative ToF-SIMS analysis. These quantitative methods will be useful for improving the physical properties of polymeric lacquer films, evaluating the lacquer quality in industry and historic conservation.

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Key words: Lacquer, Coatings, Catechols, Quantitative analysis

Visualizing Therapeutics at the Subcellular Scale by NanoSIMS

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The effectiveness of therapeutics is strongly influenced by their ability to reach the right tissues, cells, and subcellular compartments. To better understand therapeutic efficacy and potential side effects, it is essential to map their distribution within biological systems. In recent years, our lab, together with our collaborators, has developed and demonstrated a multimodal correlative imaging approach that combines light, electron, and NanoSIMS imaging, enabling the visualization of a diverse range of therapeutics at subcellular resolution in cells and tissues. We have mapped various small-molecule therapeutics containing elements with low biological background, such as iodine, bromine, and arsenic. Additionally, we have employed elemental and isotope labeling to enhance our ability to map a broader array of therapeutics in cells and tissues, including nucleic acid-based therapeutics. Our studies revealed that therapeutics target distinct subcellular compartments, and that subcellular drug compartmentalization affects overall drug efficacy.

Visualizing transient carbon storage in starch grains of pine needles by correlative AFM–nano-SIMS analysis

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Conifer forests play a major role in the global carbon cycle, yet the mechanisms governing carbon transfer and storage within needles remain poorly understood at the subcellular scale. This study aims to characterize the dynamics of assimilated carbon in pine needles under controlled conditions by combining ^{13}C isotopic labeling with high-resolution nano-SIMS imaging, with the objective of supporting future matter flux modeling.

Our experimental approach is based on pulse-chase experiments in which young pine trees are exposed to a $^{13}CO_2$-enriched atmosphere to track the fate of labeled carbon within different cellular compartments throughout day/night cycles. Particular attention is paid to starch grains, which play a central role in transient carbon storage and redistribution within the plant.

To optimize ^{13}C detection in starch grains, several sample preparation strategies were evaluated to improve both structural preservation and isotopic microlocalization. The developed methodology relies on correlative atomic force microscopy and nano-SIMS analyses, enabling the localization and quantification of isotopic enrichments at subcellular resolution.

Preliminary results demonstrate the feasibility of high-resolution isotopic mapping of assimilated carbon in conifer needles [1] and open new perspectives for the development of isotopic imaging methodologies in plant physiology.

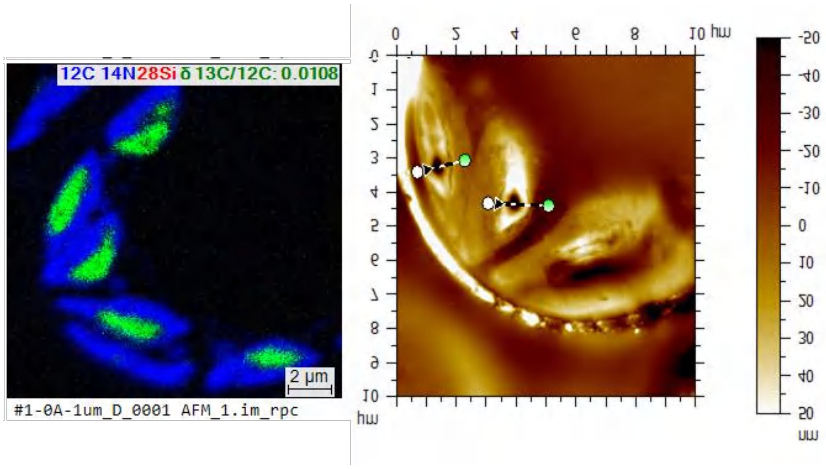


Figure 1. Localisation of ^{13}C in starch grain – SIMS and AFM images

This work was supported by the Swiss National Science Foundation (SNSF, Grant No. 214825) and the Luxembourg National Research Fund (FNR, INTER/SNF/23/17759325/microC-flux) under the Weave/Lead Agency scheme.
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Characterizing White Matter Lipid to Better Understand Demyelination and Remyelination Mechanisms during Aging

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The central nervous system (CNS), composed of the spinal cord (SC) and brain, enables information exchange throughout highly organized white matter tracts in which we find axons wrapped by a lipid-rich myelin sheath, conferring fast neurotransmission. Although the CNS can recover from demyelinating events thanks to the differentiating and regenerative abilities of oligodendrocyte precursors, this property declines with aging. Because lipids play central roles in membrane stability, cellular signaling, inflammation, and remyelination, we aim to characterize lipid dynamics in aging white matter, focusing on the dorsal SC and the corpus callosum. Recent studies highlight the importance of lipids as major regulators in the CNS [1].

To investigate age-related lipid remodeling, female C57BL/6J mice aged 2.5 months, 1, and 2 years were compared with hypomyelinated animals at postnatal day 10. Collected tissues underwent a multi-omics analysis combining ToF-SIMS, histological staining, and immunohistochemistry to highlight metabolic pathways.

Preliminary analyses confirmed the ability of ToF-SIMS to map SC and brain white matter at high spatial resolution (Fig.1). Initial observations suggest age-associated changes in lipid composition within white matter tracts. Moreover, SIMS analyses identified distinct lipid signatures associated with specific fiber tracts and sub-histological regions.

This work aims to improve our understanding of white matter lipid dynamics during aging and establish a framework for future studies of demyelination and remyelination in disorders such as multiple sclerosis [2].

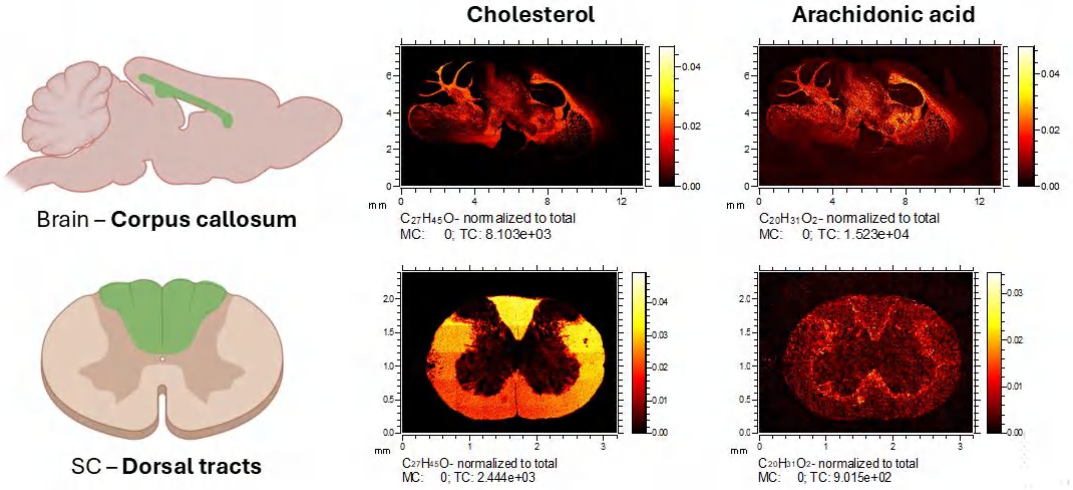


Figure 1. Illustration of our region of interest and chemical information obtained by ToF-SIMS analysis. Cholesterol is a major component of myelin, and arachidonic acid plays multiple roles in the CNS.

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Effect of Ketogenic Diet on Brain Lipid Composition Investigated by ToF-SIMS Imaging and Multivariate Analysis

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The ketogenic diet (KD) induces substantial metabolic changes; however, its influence on brain lipid composition remains incompletely understood. This study aims to investigate diet-induced alterations in lipid profiles in rat brain cortex tissue using time-of-flight secondary ion mass spectrometry (ToF-SIMS) combined with multivariate analysis. ToF-SIMS imaging, performed in both positive and negative ion modes, enables label-free, high spatial resolution analysis of molecular distributions in biological tissues. This approach provides complementary information on lipid species, including fatty acids, cholesterol, and phospholipid-related fragments, allowing for detailed characterization of biochemical changes. Brain samples from four groups—ketogenic females (KF), ketogenic males (KM), normal diet females (NF), and normal diet males (NM)—were analyzed. Key lipid species, including cholesterol-related ions ($C_{27}H_{45}^+$, $C_{27}H_{45}O^+$), fatty acids, and phospholipid-related fragments, were identified and semi-quantified. Statistical analysis revealed significant differences in cholesterol-related signals, with consistently lower intensities observed in ketogenic groups compared to controls. Importantly, these differences were driven primarily by diet rather than sex. The ratio of cholesterol fragment ions (m/z 385/369) indicated a shift toward increased free cholesterol in KD groups, while esterified cholesterol was more abundant in animals on a standard diet. Principal component analysis (PCA) demonstrated clear separation between ketogenic and control groups, confirming the dominant influence of diet on biochemical composition. In addition to cholesterol-related changes, a chain-length-dependent remodeling of fatty acids was observed. Medium-chain fatty acids (e.g., C10 and C14) were enriched in ketogenic samples, whereas long-chain fatty acids (C16 and C18) were more abundant in controls, consistent with increased fatty acid utilization under ketogenic conditions [1]. Furthermore, reduced ratios of unsaturated to saturated fatty acids (C18:1/C18:0 and C18:2/C18:0) were observed in ketogenic samples, indicating decreased desaturase activity and enhanced lipid utilization. These findings demonstrate that the ketogenic diet induces coordinated changes in cholesterol metabolism and fatty acid composition, leading to lipid remodeling in the brain. The combined effects of altered chain length distribution, reduced desaturation, and changes in cholesterol balance may influence membrane organization, fluidity, and neuronal function. These findings demonstrate the potential of ToF-SIMS imaging combined with multivariate analysis for spatially resolved brain lipidomics.

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Water Cluster Advances for Biological SIMS: From Beam Chemistry to Cryogenic Conditions

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Low ionisation yields remain one of the central challenges in SIMS analysis of biological materials. Numerous strategies have been explored to address this, including matrix addition, metal coating, and laser post-ionisation. Among the most promising approaches is the introduction of proton-donating molecules, either directly to the sample, the surrounding atmosphere, or the ion source. Water has proven to be a particularly attractive candidate as it is inexpensive, safe, and effective at enhancing ionisation efficiency. The adoption of water gas cluster ion beams (GCIB) has delivered significant benefits, both improving ionisation yields and reducing matrix effects [1]. Further work on doping these clusters with reactive gases has amplified these beneficial effects [2], and allowed for analysis of multiply charge small proteins [3]. This also translated to increased yield and improved imaging capabilities for cholesterol which has historically proven difficult to ionise and analyse using mass spectrometry techniques [4]. Cryogenic analysis is important for maintaining morphology and localisation in high resolution tissue imaging and as a means of better preserving sample chemistry [5]. Our research is investigating the fundamental parameters that determine to what extent large water clusters affect sputter and ionisation efficiency, and what role cryogenic conditions might play in this process.

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Molecular dynamics of gas cluster sputtering of peptides: Influence of the sample and cluster nature

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Secondary ion mass spectrometry is very efficient to identify and localize organic and biomolecules in solid samples via 2D and 3D imaging, allowing the analysis of biosurfaces such as polymer blends, protein assemblies, tissue sections and even single cells. In support to the experiments, this study explores the differences in fragments, molecules and cluster distributions emitted from peptidic layers on gold using reactive molecular dynamics simulations. The nature of the systems varies, from monolayers to multilayers on gold and water-matrix embedded peptides, similar to frozen-hydrated samples in Cryo-SIMS. The research first highlights how layer thickness influences the fragmentation of the hormone glucagon (Figure 1): monolayer sputtering results in intense fragmentation while multilayers enable softer sputtering, ejecting larger fragments, intact molecules and clusters, as was previously observed with larger enzymes [1,2]. Notably, new polypeptide structures may arise from glucagon molecule recombination during sputtering, altering amino acid sequences while maintaining backbone connectivity. We then analyze the differences between the dynamics of emission from pure glucagon multilayers and glucagon embedded in a water matrix. Finally, our simulations explore the effects of varying the cluster nature, from Ar to H_2O. The findings underscore the critical roles of the peptide sample structure, projectile nature and surface interactions on the fragmentation and emission dynamics, offering insights for improved protein sequencing and identification by SIMS.

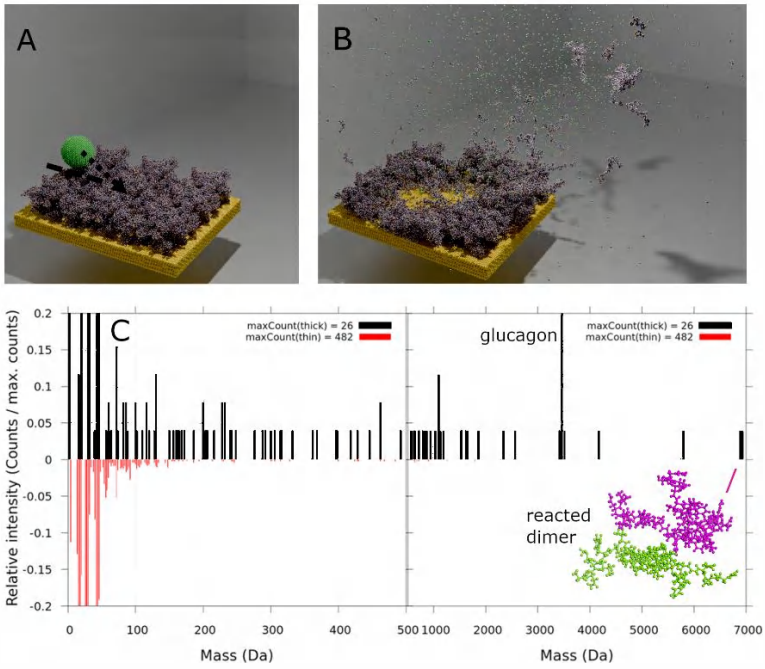


Figure 1. (A-B) 20 keV Ar3000-induced emission from a glucagon thick layer; (C) Comparison of the mass spectra computed from thick (black) and thin (red) layers.

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Water-assisted SIMS using Gas Cluster Ion Beams

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An increase in secondary ion yields with a reduction in impact-induced chemical damage for Secondary ion mass spectrometry (SIMS) has been a primary focus for many years. A number of approaches have been adapted including the introduction and then further modification of gas cluster ion beams (GCIBs) [1-3] as well as an analysis of the samples within an ice matrix [4].

Here, we present a novel methodology of using water-GCIBs as a highly-controlled method to deposit water ice on non-hydrated samples as a means of enhancing SIMS performance using a second, more focused, primary ion beam such as C_{60}. Preliminary data from glucose and adenosine triphosphate (ATP) samples show an increase in molecular ion yields by a factor x10-100, Figure 1. The effect is sensitive to sample temperature, water cluster velocity, and dose [5] but the level of enhancement exceeds that reported previously for gas-phase water dosing in vacuum [6].

The methodology, termed 'water-assisted SIMS', may be particularly useful for samples that cannot be prepared in a frozen-hydrated state or where the desired lateral resolution of the SIMS analysis exceeds that of a reactive gas cluster ion beam such as $(H_2O)_n$.

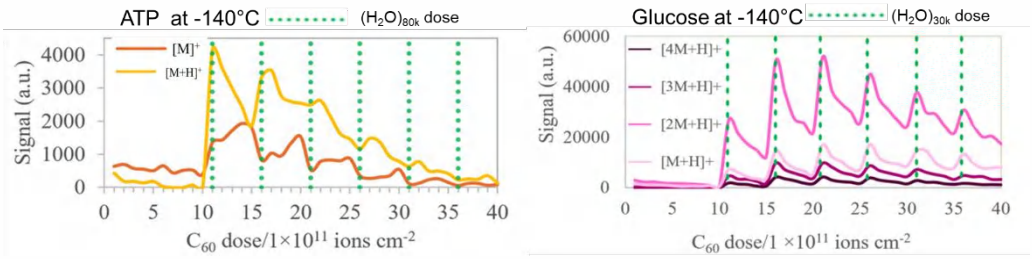


Figure 1 - Illustrates the enhancement of water-GCIB dosing on the C60-SIMS analysis of a molecular surface.

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Comparative Study on Desorption Mechanisms between Ar- and water-GCIB Irradiation on Organic Thin Films

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1. Introduction

Water-GCIB-ToF-SIMS significantly enhances organic molecular ion yields compared to Ar-GCIB [1], but the underlying mechanisms remain unclarified. We investigated the energy-per-constituent-molecule (*E*/*n*) dependence of secondary ion formation using benzylpyridinium (BP) thermometer ions to probe internal energy deposition during cluster impacts.

2. Experimental

An aqueous solution of 1-(4-nitrobenzyl)pyridinium chloride (1 g/L) was drop-cast onto Si substrates and vacuum freeze-dried. Ar- and D_2O-GCIBs were operated at an acceleration voltage of 5 kV, with cluster sizes (n) ranging from 500 to 3000, thereby precisely controlling *E*/*n* from 1.7 to 9.6 eV.

3. Results and Discussion

The *E*/*n* dependence of intact molecular cation (M^+, *m*/*z* 215) and D_2O-adduct yields was comparatively evaluated (Figure 1). In the low *E*/*n* region below 2 eV, both clusters showed a sharp increase in M^+ yield, suggesting that the cluster kinetic energy effectively dissipates into the bulk film, leaving insufficient recoil energy for the analyte molecules to desorb [2]. However, while the Ar cluster yield plateaued above 2 eV, the D_2O cluster yield rose steeply, peaking at ~3 eV before declining. Crucially, D_2O-adduct ions were exclusively detected at *E*/*n* < 3 eV, matching the yield enhancement regime. This strong correlation demonstrates that co-desorbed water molecules induce a soft-ionization and cooling effect, effectively stabilizing the molecular ions within the high-density ablation plume.

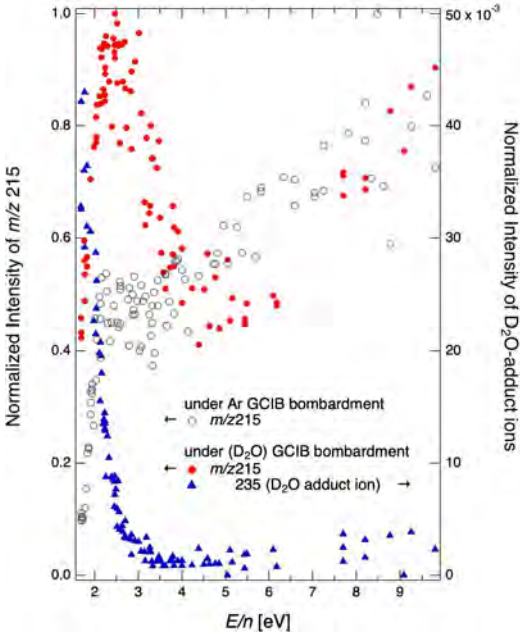


Figure 1 E/n dependence of the yields for the *m*/*z*215 ions and the corresponding D_2O adduct ions. The vertical axis is normalized with the maximum intensity for each species.

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Secondary Ion Mass Spectrometry of Amino Acids and Explosives by Electrospray Droplet Ion Beams

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We have been studying electrospray droplet ion (EDI) beams as novel massive cluster ion beams for secondary ion mass spectrometry (SIMS) [1,2]. Atmospheric pressure and vacuum electrosprays of H_2O/CH_3OH solutions containing 0.01 M trifluoroacetic acid were used for EDI beam generations. Fragmented secondary ions were suppressed by using the EDI beams and intact molecular ions were produced with high intensities. In this study, SIMS analyses by the EDI beams were applied to amino acids and explosives [3,4].

For the explosives of HMTD (hexamethylenetriperoxidediamine), RDX (cyclotrimethylene trinitroamine), HMX (cyclotetramethylenetetranitroamine), PETN (pentaerythritol tetranitrate), and TNT (2,4,6-trinitrotoluene), intact molecules were produced by the EDI beams. Nitramines of RDX and HMX were detected as H^+ and Na^+ adduct ions with H_2O and CH_3OH ligands. TNT and PETN related ions were not found in positive mode. In negative mode, RDX, HMX and PETN were detected as adduct ions with NO_2^-, NO_3^-, and CF_3COO^-. TNT gave $TNT^{-\bullet}$ and fragment ions similar to those detected in atmospheric-pressure chemical ionization.

For the essential amino acids (AAs), cluster ions of AAs were formed by the EDI beams both in positive and negative modes. The AA cluster ions have been also reported to be formed by Argon gas cluster ion beams [5]. For AAs with apolar side chains such as Ala and Val, Leu, and Ile, while large sizes of positive cluster ions $[n(AA)+H]^+$ (n=11–21) were observed, negative cluster ions $[n(AA)–H]^-$ were observed with only n up to 3. The AAs with polar side chains (Ser, Thr, Asn, Gln, Tyr and Cys) gave similar n up to 7–12 for both $[n(AA)+H]^+$ and $[n(AA)–H]^-$. For basic AAs (Lys and Arg), the maximum n values observed for $[n(AA)+H]^+$ are larger than those for $[n(AA)–H]^-$ and vice versa for acidic AA (Asp and Glu). The stability of AA cluster ions appears to be strongly affected by the polarities and structures of amino acids.

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Mass spectroscopy in molecular resolution:

Atom probe tomography of polymers and complex fluids

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Atom probe tomography is a method of microscopic analysis well-established in the study of hard materials. It is based on the controlled field desorption of individual atoms or small molecular fragments from nanometric specimens and stands out by combining single-atom sensitivity with a 3D volume reconstruction in sub-nanometer resolution. A particular stronghold of the method is the accurate measurement of chemical segregation at grain boundaries and interfaces in complex nanostructured matter.
Our current efforts concern advanced volume reconstruction schemes, the simulation by first-principles methods of the evaporation process [1] and a full statistical understanding of chemical fluctuations in the data sets [2]. Most recently, we desire to break the materials limitations towards the analysis of soft matter and polymeric materials with this method [3].

In order to investigate the structure of complex fluids and soft materials, micro-droplets of liquids are quench-frozen in tiny metallic beakers cut into tungsten tips and then after freezing, the liquids are shaped with focused ion beams into nano-needles. These needles are transferred into the atom probe measurement chamber without melting. Meanwhile, we investigated with this method, aqueous solutions, alkanes and organic solvents as well as complex molecular liquids such as liquid crystals.

Usually, the time-of-flight mass spectra of organic liquids are quite complex containing a variety of small to large fragments. Nevertheless, by accurate fitting procedures, a peak assignment and correct quantitative interpretation becomes often possible. The talk focuses on the issue of volume reconstruction. We present an advanced scheme of reconstruction, that takes into account frequent deviations from the required ideal hemispherical sample shape. In order to clarify whether the obtained reconstructions of polymeric materials and disordered liquids may contain reliable spatial information, we apply next-neighbor statistical methods and fluctuation analysis. i) By evaluating fluctuations of the local chemical environment, order/disorder tendencies are identified and even the Gibbs energies of mixture can be quantified. ii) Similarly, fluctuation analysis is a helpful tool to check the accuracy of positioning atomic species in the volume reconstructions. Statistical next-neighbor analysis is proposed to reveal structural aspects of amorphous polymers or mixtures of amino acids. As examples, measurements of carnosine in aqueous solution as well as of polyvinylpyrrolidone (PVP) will be presented.

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Atom Probe Tomography Reveals Tungsten-Mediated Atomic-Scale Stabilization of Hierarchical Microstructures in Ni-Based High-Entropy Superalloys

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High-entropy superalloys (HESAs) combine the core effects of multicomponent alloys with the precipitation-strengthened architecture of conventional superalloys, thereby exhibiting excellent elevated-temperature mechanical properties. A key challenge in HESA structural design is the thermal stability of the hierarchical $\gamma_m \supset \gamma' \supset \gamma_p$ microstructure, in which nanoscale γ_p are prone to coarsen, split γ', or dissolve at high temperatures. In this study, atom probe tomography (APT) was employed to investigate how tungsten (W) content influences phase stability in the NiCoAlFeCrTiNbMoWx alloy series through atomic-scale mechanisms.

After homogenization at 1500 K for 44 h, alloys containing 0.4, 0.6, and 1.0 at.% W were aged at 1023 K for 5, 10, 20, 100, 200, and 400 h. APT analyses were performed on the homogenized alloys and on alloys aged for 5 and 100 h to quantitatively track elemental partitioning behavior and cluster evolution across the γ_m/γ' and γ'/γ_p interfaces. The main findings are as follows: (1) Cr-enriched nanoclusters within the γ' phase resolved by APT serve as nucleation precursors for γ_p, and increasing W content tends to produce fewer but larger clusters; (2) W exhibits opposite partitioning tendencies across the two interfacial systems: in the γ_m/γ' system, W preferentially partitions to the γ matrix, whereas in the γ'/γ_p system, W preferentially partitions to γ'; (3) increasing W content raises the mixing Gibbs free energy (G_{mix}) of the γ', thereby enhancing the thermodynamic driving force for γ' to γ_p phase separation, while simultaneously slowing coarsening kinetics owing to the low diffusivity of W.

This study demonstrates atomic-scale partitioning and clustering dynamics in compositionally complex alloys, providing quantitative atom-by-atom insights into the thermodynamic stabilization of hierarchical precipitate structures. The results establish a design framework for developing thermally stable HESAs for high-temperature structural applications through refractory element alloying.

Influence of Atom Probe Tomography Measurement Conditions on the Compositional and Spatial Distribution Analysis of $LiNi_{0.5}Mn_{1.5}O_4$ Cathode Materials

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Accurate characterization of elemental composition and three-dimensional cation distribution is a fundamental prerequisite for unraveling the degradation mechanisms of cathode materials during electrochemical cycling. Atom probe tomography (APT) enables quantitative analysis of multi-element distributions in electrode materials at the nanoscale; however, the reliability of its compositional and microstructural results is highly susceptible to experimental measurement conditions. In this work, APT was employed to systematically characterize pristine spinel $LiNi_{0.5}Mn_{1.5}O_4$ (LNMO) cathodes under a range of experimental parameters, including laser pulse energies of 5 pJ, 10 pJ, and 20 pJ, as well as different detection rates. The results demonstrate that measurable, albeit slight, deviations in cation stoichiometric ratios are observed across different laser energy conditions, confirming that APT measurement parameters exert non-negligible effects on quantified elemental contents. This finding provides a direct reference for stoichiometry calibration in subsequent APT analyses of both pristine and cycled LNMO samples. Meanwhile, experimental conditions are found to alter the apparent spatial distribution and homogeneity of constituent elements. This result is critical for distinguishing measurement-induced inhomogeneity artifacts from genuine structural degradation arising from electrochemical cycling in future characterizations. In addition, oxygen loss, a well-documented challenge in APT analysis of oxide cathode materials, was detected under all tested conditions. This study systematically elucidates the effects of APT experimental parameters on the agreement between measured elemental stoichiometry and the theoretical formula, as well as the spatial distribution uniformity of LNMO. It establishes a methodological foundation for more accurate and reliable APT characterization of high-voltage spinel cathode materials.

Key words: APT, LNMO, Cathode,

High-Resolution Magnetic Sector SIMS for Advanced Semiconductor and Materials Science Applications

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The increasing miniaturization as well as structural and chemical complexity of advanced materials and semiconductor devices raises the need in analytical techniques that offer high spatial resolution, high elemental sensitivity, and precise navigation across multilayer architectures.

The IONMASTER magSIMS system addresses these requirements through a high-brightness liquid metal alloy ion source allowing to bombard the sample with heavy primary ions such as Au^+ or Bi^+ enabling efficient sputtering with high secondary ion yields with sub-25 nm spatial resolution. High transmission (> 40 %) secondary ion optics are combined with a magnetic-sector mass analyzer and a continuous focal plane detector leading to high elemental sensitivity (e.g., < 10 ppm for Li). The focal plane detector allows full-spectrum recording at every image pixel without duty cycle. A laser-interferometer stage that ensures single-digit-nm precise sample navigation [1].

Furthermore, one key capability of the platform is its capability of an automated navigation workflow using coordinate-based navigation in combination with high-resolution SIMS analysis. The system supports KLARF based wafer map import as well as GDSII driven structure targeting, including guided site-specific SIMS analysis with a high throughput across complex semiconductor layouts.

We present here case studies that highlight the key capabilities of the IOMASTER with examples from materials science and semiconductor analysis workflows, including high-resolution SIMS imaging of an Infineon 16 MB DRAM microchip (Fig. 1).

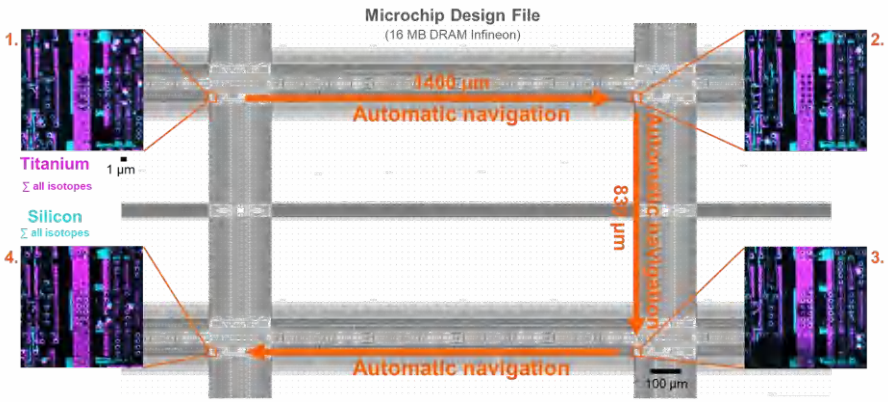


Fig. 1. Automatic nm-precise sample navigation workflow with subsequent high-resolution SIMS imaging of a 16 MB DRAM Infineon microchip. Recorded SIMS maps of Titanium and Silicon are shown in magenta and cyan, respectively.

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Understanding Dynamic SIMS with Magnetic-Sector Instruments: From Fundamentals to Practical Use

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Secondary Ion Mass Spectrometry (SIMS) comprises a range of analytical modes that address different scientific and industrial challenges. While static SIMS is widely used for molecular and surface-chemistry analysis, dynamic SIMS, particularly when implemented on magnetic-sector instruments, remains the reference technique for quantitative elemental and isotopic characterization. This tutorial is designed to introduce dynamic SIMS in a clear and pedagogical manner, specifically for SIMS users who are less familiar with this approach.

The session begins with a review of SIMS fundamentals, emphasizing the distinction between static and dynamic regimes in terms of primary ion dose, sputtering behavior, and analytical outputs. In dynamic SIMS, a continuous focused primary ion beam (typically O_2^+ or Cs^+) is used to sputter material under controlled conditions, enabling reproducible depth profiling and highly sensitive analysis. The formation and extraction of secondary ions are described step by step, followed by an introduction to magnetic-sector mass analyzers and their advantages in terms of high transmission, high mass resolving power, and signal stability.

Key performance metrics of dynamic SIMS will be explained in an instructional manner, including trace detection limits (from ppm to ppb levels), depth resolution (down to the sub-nanometer scale), high-precision isotopic ratio measurements (down to the 0.1 ‰ range), and imaging capabilities with lateral resolution down to tens of nanometers. The tutorial will illustrate how these capabilities enable one-dimensional depth profiles, two-dimensional elemental or isotopic maps, and three-dimensional elemental reconstructions, and how they complement other microanalytical techniques.

Practical aspects of dynamic SIMS analysis will be addressed, including primary ion species selection, matrix effects, charge compensation strategies, quantification approaches, and basic data interpretation. Representative case studies from semiconductor device structures and other advanced materials will illustrate how CAMECA magnetic-sector SIMS instruments are applied in both research environments and routine process control.

This tutorial is intended for SIMS users who wish to broaden their analytical toolbox and gain a clear understanding of when and how dynamic SIMS with magnetic-sector instruments provides decisive advantages. By the end of the session, attendees will have a solid conceptual framework for dynamic SIMS and a practical appreciation of its capabilities within the broader SIMS landscape.

Correlative High-Resolution Surface and Mineralogical Imaging of a South American Ion-Adsorption Rare Earth Deposit Using ToF-SIMS, XPS, and Automated Mineralogy

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Ion-adsorption clay (IAC) deposits are increasingly important for diversifying global rare earth element (REE) supply, yet their economic processing depends critically on understanding REE occurrence at both the particle and surface scale. Here, we present a correlative high-resolution imaging and spectrometry workflow combining time-of-flight secondary ion mass spectrometry (ToF-SIMS), X-ray photoelectron spectroscopy (XPS), and automated mineralogical mapping (QEMSCAN/TIMA-X-type analysis) to resolve REE deportment and surface binding environments within a South American IAC material.

Bulk mineralogy indicates a matrix dominated by kaolinite and mica-rich clays, with minor quartz and Fe-oxide/oxyhydroxide associations, while automated mineralogy identifies monazite as the primary discrete REE mineral (~0.26–0.28 wt%) and provides statistically robust liberation and association metrics. Liberation of monazite increases substantially in the fine fraction (from ~32% in <300 μm to ~65% in <50 μm), indicating that targeted size classification could enable effective pre-concentration prior to chemical processing. Importantly, mineral deportment calculations reveal a pronounced decoupling of REEs: Ce is largely hosted in monazite and REE-phosphate phases, whereas Y is predominantly associated with clays/micas, implying that physical recovery of monazite alone may leave significant heavy REE value in the silicate fraction [1].

Surface-sensitive analyses provide direct evidence for REE occurrence at the outermost surface. XPS surveys show Al- and Si-dominated silicate surfaces with trace transition-metal oxyhydroxides, consistent with clay-hosted adsorption environments. ToF-SIMS chemical imaging detects Nd and Dy ions distributed as thin surface layers, supporting an ion-adsorbed or surface-complexed mode of occurrence. Together, ToF-SIMS and XPS bridge the gap between mineral-scale deportment and nanoscale surface chemistry, enabling a mechanistic basis for selecting ion-exchange leaching strategies while informing the role of refractory REE phases [1].

This integrated HR imaging/spectrometry approach demonstrates how combining ToF-SIMS, XPS, and automated mineralogy can resolve REE partitioning across phases and surfaces, providing critical insight for designing hybrid beneficiation–leaching flowsheets for emerging IAC resources.

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Towards Molecular Volume Imaging with Sub-cellular Resolution

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Volume imaging techniques such as cryogenic focused ion beam electron microscopy (cryo-FIB-SEM) reveal exquisite 3D biological structure of biological material [1,2]. However, there is no molecular information, which would provide powerful complementary insight. In 2017, we introduced the OrbiSIMS technology [3] bringing the performance of an Orbitrap mass spectrometer together with the high-resolution imaging capability of SIMS [4]. We were able to map the distribution of lipids and neurotransmitters in mouse brain with sub-cellular resolution. We also demonstrated the ability for single-cell metabolic profiling of macrophage cells incubated with the anti-arrhythmia drug, amiodarone, revealing strong heterogeneity of drug uptake. However, with single-cell resolution a clear correlation of drug uptake with upregulation of specific lipids was found. The unique ability of OrbiSIMS to simultaneously provide high-confidence in a molecule's location and identity has led to strong uptake in a wide range of science and technologies, with now many instruments installed worldwide.

Inspired by advances in Cryo-EM, we introduced the cryo-OrbiSIMS which allows imaging in the native biological state [5]. For example, we demonstrated the ability to undertake in-situ metabolomics of biofilm formation and in collaboration with the Francis Crick Institute we mapped the distribution of metabolites on the cuticular surface of drosophila. [6] We are now combining cryo-OrbiSIMS with an in situ cryo-FIB to develop protocols for molecular volume imaging. Initial results will be presented as well as novel routes to improve Orbitrap data analysis.[7]

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The lifespan of the Moon

Qiu-Li Li[1,2], Mu-Han Yang[1,2], Qian W.L. Zhang[1], Bi-Wen Wang[1], Xian-Hua Li[1,2]

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The fundamental questions of when the Moon formed and how long its internal geological activity persisted remain central to planetary science. Recent analyses of returned lunar samples and lunar meteorites have dramatically extended the record of lunar volcanism. Key findings include young mare basalts on the lunar nearside (~2.0 Ga)[1], farside basalts (~2.8 Ga)[2], a ~2.2 Ga KREEP-enriched basaltic lunar meteorite[3], and crucially, volcanic glass beads indicative of volcanic activity as recent as ~120 Ma[4]. These discoveries collectively point to a Moon with sustained endogenic geological vigor far longer than previously recognized.

To constrain the earliest lunar history, we employ a two-stage Pb isotope evolution model on four precisely dated mare basalt samples with well-defined initial Pb isotopic compositions. Our modeling calculates the timing of mantle source homogenization for these mare basalts to be ~4377 +57/-27 Ma. Extrapolating this model further back in time allows us to estimate the age of the Moon's primary differentiation, which we interpret as the lunar formation time, at ~4516 +21/-18 Ma[5].

This study provides chronological constraints from the Moon's late-stage volcanic products to its very origin. The results reconcile a formation time of the Moon within the context of the Giant Impact hypothesis with newly recognized evidence for its extraordinarily prolonged volcanic history.

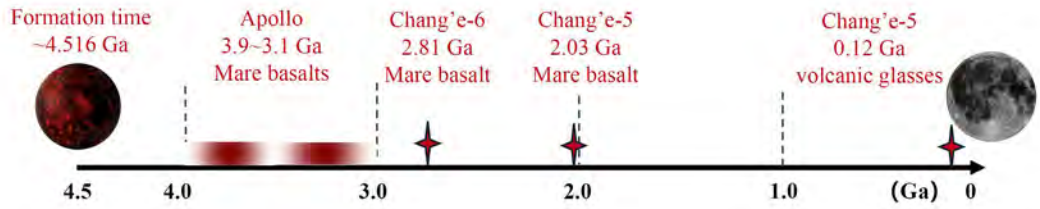


Figure 1. The lifespan of lunar volcanism. Ga = billion years ago

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Correlated Laser Ionization/TOF-SIMS Imaging Mass Spectrometry with Continuous C60 Ion Beam

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Secondary ion mass spectrometry, as a powerful surface analysis tool, is widely used in semiconductor and geoscience applications. Especially, with the advancement of cluster ion source technology, TOF-SIMS has received widespread attention in biochemical imaging, such as spatially resolved metabolomics research. However, despite the high sensitivity and excellent spatial resolution of SIMS, relying solely on the m/z information of the secondary ions is difficult to describe the sample surface information, including chemical valence state, pathological features, and surface morphology. Correlated technologies such as Raman/infrared spectroscopy, optical microscopy, electron microscopy SEM, and MALDI can complement the SIMS technology well. In recent years, correlated imaging technologies and instruments have attracted strong interested.

In this work, we have constructed a correlated laser ionization/TOF-SIMS imaging mass spectrometry with continuous C_{60} cluster primary source. The instrument including the C_{60} ion beam, Schwarzschild optical microscope, ion extraction and transfer system and W-TOF mass analyzer. Schwarzschild microscope features a large numerical aperture (NA=0.47), a 50 mm working distance, and excellent coordination with the ion extraction system. A spatial resolution of 0.7 μm has achieved, with an imaging field of view of 300 μm * 400 μm, primarily utilized for sample navigation and micro-area positioning. The ion transfer system consists of three-stage quadrupoles, enabling ion cooling, mass filtering, and ion enrichment. Currently, the mass resolution of TOF-SIMS has reached 15,000. The microscope imaging and mass imaging of the 200-mesh molybdenum mesh and Indium foil surface are shown in Figure 1(b) and (c), respectively.

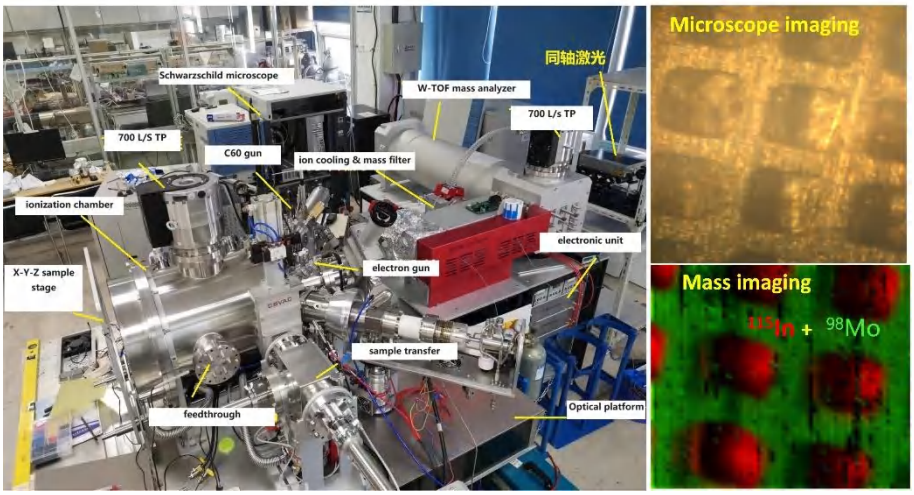


Figure 1. (a) Instrument overview of the correlated microscope/SIMS imaging mass spectrometry. (b)Microscope imaging of the 200-mesh molybdenum mesh and Indium foil surface. (c) Mass imaging of the 200-mesh molybdenum mesh(green) and Indium foil surface(red).

Multi-resolution MALDI-MSI platform with Integrated MALDI-2

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Matrix-assisted laser desorption/ionization mass spectrometry imaging (MALDI-MSI) enables spatially resolved molecular analysis of biological tissues, but achieving both high spatial resolution and high sensitivity remains challenging. Here, we present a novel dual-mode MALDI-2 ion source coupled to an Orbitrap mass spectrometer that combines transmission and reflection laser geometries with enhanced ion transmission for high-resolution molecular imaging.

The source integrates reflection MALDI (~20 µm spatial resolution) and transmission MALDI (~2 µm spatial resolution), enabling flexible imaging across multiple length scales. A secondary 260 nm MALDI-2 laser provides gas-phase post-ionization to increase ion yields, while a newly developed intermediate-pressure ion optics system generates laminar gas flow, suppresses turbulence, and minimizes ion diffusion during transport. The platform was coupled to a Thermo Scientific Orbitrap Elite mass spectrometer, providing high mass resolving power and mass accuracy for molecular imaging applications.

System optimization included matrix deposition protocols, laser fluence, optical alignment, and ion-transfer conditions. Imaging experiments performed on biological tissue sections demonstrated sub-5 µm ablation performance and improved ion transmission efficiency. MALDI-2 significantly enhanced sensitivity across a broad range of lipid classes compared with conventional MALDI. In mouse brain tissue coated with 2,5-dihydroxyacetophenone (DHA), MALDI-2 generated substantially increased lipid signal intensities and enabled detection of low-abundance species. Transmission MALDI produced high-resolution molecular images revealing fine tissue features, while reflection MALDI enabled rapid large-area analysis. Furthermore, tandem MS experiments acquired in data-dependent acquisition mode supported confident lipid identification directly from imaging experiments.

These results demonstrate that the combination of dual-mode MALDI, MALDI-2 post-ionization, and improved ion-transfer optics enables sensitive, high-spatial-resolution molecular imaging on an Orbitrap platform. The approach expands the analytical capabilities of MALDI-MSI and provides a versatile tool for applications in cellular biology and spatial omics research.

Modification of microbeam Cs ion source

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(3) Hokkaido univ.

Cesium ions are important for primary beam of Secondary Ion Mass Spectrometry. Cs metal is burnable and is difficult for use. Some provider of SIMS instruments adopt compound Cs source instead of pure Cs metal. In case of Cameca instruments Cs2CO3 is utilized for producing Cs gas in their ion gun. The gun consists of two parts; ionizer and reservoir. High volage is applied on both parts and they are heated by electron bombardment. The electron is coming from heated filaments surrounded with them. The power is regulated by emission current from the filament. Cs3CO3 is packed inside reservoir part. It is heated not only electron bombardment but also radiation from the filament and heat conduction from ionizer part. In fact, we can obtain high ion current even though the current of reservoir filament is zero, especially with new source. The filament current is required about 5 A or higher to generate thermal electron. This means that we cannot control reservoir temperature in some range.

In this work we have tried to heat the reservoir part only radiation from the filament; with filament current from 0 A to 5 A. As a result, stable high ion current was realized. We also have made Cs ionizer by ourselves in order to reduce the volume of ionizer part. Using this ionizer, we obtained enough Cs ion current with emission current of 1.3 mA for ionizer part. It is lower than the typical value of ims 7f (1.85 mA). It would be useful if energy of primary ions was reduced.

Quantitative Description of Ion Implantation Profile Based on Pearson Distribution

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Ion implantation is a critical process in semiconductor manufacturing, where precise control over dopant profiles is essential for achieving desired device performance. However, implantation profile varies with many factors, such as substrate crystalline and its orientation, implantation conditions like energy, incident angle and divergent angle etc. Commonly used Gaussian profile may deviate from the real implantation profile. This study introduces Pearson distribution to quantitatively describe ion implantation profiles. We validated this approach with several typical ion implant profiles. Moreover, we applied the approach to successfully identify the root causes of implanter failures, such as energy and angle shifts, which can adversely impact implantation precision. This methodology provides an accurate tool matching and accurate TCAD simulation, enhancing process reliability and device yield in advanced semiconductor design and fabrication.

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Key words: ion implantation, dopant profile, Pearson distribution, quantitative description

Identifying Low-alpha Solder via Lead Isotope Fingerprint using ToF-SIMS

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Alpha-particle emission from solder materials presents a critical reliability concern in electronic packaging, particularly for microelectronic devices susceptible to soft errors induced by radioactive decay. While low-alpha particle (LAP) solders are widely employed to mitigate this risk, distinguishing them from standard non-LAP solders remains a significant challenge. Conventional direct alpha-particle emission measurements are often time-consuming and cost-prohibitive, rendering them impractical for rapid materials screening. To address this limitation, this study proposes a novel lead (Pb) isotope fingerprinting method utilizing Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) to identify LAP solder through geological source tracing. Because stable lead isotopes preserve information from long-term radioactive decay systems, ^{206}Pb, ^{207}Pb, and ^{208}Pb serve as the stable end products of uranium (U) and thorium (Th) decay chains, while ^{204}Pb provides a non-radiogenic reference baseline. Consequently, isotope ratios-specifically $^{206}Pb/^{204}Pb$, $^{207}Pb/^{204}Pb$, and $^{208}Pb/^{204}Pb$-can distinguish lead sourced from different geological mines, acting as characteristic provenance fingerprints for the solder.

In this work, ToF-SIMS was first utilized to analyze six commercial high-lead solder samples of known alpha-particle grades, establishing a foundational lead isotope fingerprint reference map. Commercially sourced, unknown solders within microelectronic packages were subsequently characterized using the same protocol. Notably, the isotope fingerprints of these unknown solders aligned with distinct regions on the pre-established reference map, enabling the accurate differentiation between LAP and non-LAP solders. To validate these findings, independent alpha-particle emission reliability tests were conducted, yielding consistent and supportive results. Ultimately, this work demonstrates a rapid, high-precision method for identifying low-alpha solder via ToF-SIMS-based lead isotope fingerprinting. Future efforts will focus on expanding the reference database with a broader range of solder samples to further solidify the classification model.

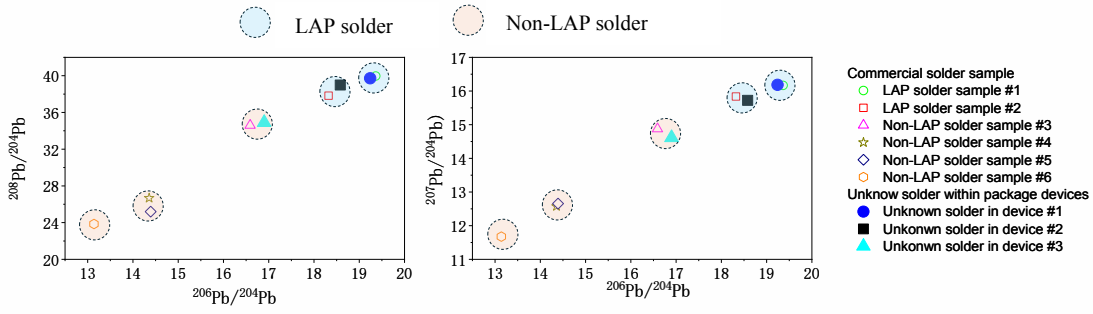


Figure 1. Lead isotope fingerprint reference map of solders used in microelectronic packages.

Quantitative Comparison of Trace Impurities in Cu Thin Films via Oxygen-Controlled D-SIMS Analysis

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Copper (Cu) thin films are widely used as interconnect materials in semiconductor devices due to their excellent electrical conductivity. However, impurity incorporation during processing and handling can degrade electrical and interfacial properties, leading to reduced device performance and reliability. As device scaling advances, accurate evaluation of trace impurities has become increasingly important.

Dynamic secondary ion mass spectrometry (D-SIMS) is a powerful technique for trace impurity analysis; however, in Cu films, oxygen strongly affects secondary ionization, making quantitative analysis and sample comparison difficult. Variations in oxygen concentration alter ionization yield, causing fluctuations in signal intensity even for the same element. As a result, direct comparison of impurity levels between samples with different oxygen contents is challenging.

To investigate this issue, Cu samples with different oxygen conditions were prepared: (1) a continuously deposited 60 nm Cu film, (2) a film with a 30 nm deposition followed by 100 s air exposure and an additional 30 nm deposition. In sample (2), signal intensities of hydrogen, carbon, and fluorine increased due to oxygen incorporation, making comparison difficult.

To overcome this, the oxygen leak method was applied using a Cs primary ion beam. By introducing oxygen to homogenize surface conditions, matrix effects were reduced, enabling reliable comparison of trace elements across samples.

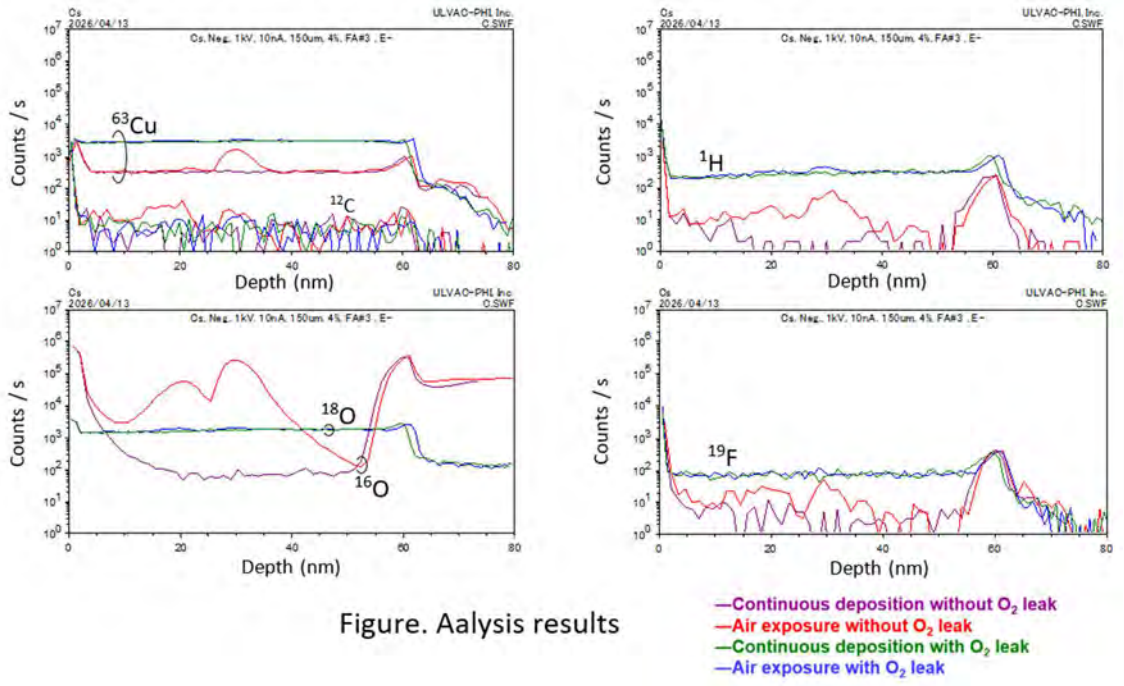


Figure. Aalysis results

Comprehensive SIMS Characterization for Dopant Profiling and Carrier Distribution in Wide Bandgap Semiconductor

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Wide bandgap semiconductor materials (SiC, GaN, AlGaN, etc.) are increasingly being applied in high-power and high-frequency electronic devices. Precise characterization of dopant elements and accurate measurement of carrier distribution are critical to ensuring device performance and reliability. Secondary Ion Mass Spectrometry (SIMS) technology, with its extremely high detection sensitivity (ppb level) and excellent depth resolution, combined with complementary characterization techniques such as Scanning Capacitance Microscopy (SCM) and X-Ray Diffraction (XRD), provides an irreplaceable comprehensive characterization solution for dopant process optimization and device structure verification of wide bandgap semiconductor materials.

This presentation will systematically introduce the latest application progress of SIMS and its combined techniques in the characterization of wide bandgap semiconductor materials, with a focus on: SIMS quantitative analysis of N and Al doping in SiC materials; SIMS characterization of Al doping; SIMS combined with SCM for carrier distribution characterization in SiC super junction and deep trench structures; SIMS characterization of H, Mg, and C doping in GaN HEMT structures; and SIMS combined with XRD for AlGaN composition and doping characterization. Key challenges in SIMS analysis will be discussed, including matrix effect correction, factors influencing detection limits, and data correlation and consistency verification strategies when employing multiple combined techniques. Through characterization case studies of specific device structures (SiC high-voltage epitaxial structures, SiC super junctions, deep trench MOSFETs, and GaN HEMT heterostructures), this presentation will demonstrate how SIMS and its combined techniques provide systematic characterization solutions for dopant process optimization, device structure verification, and reliability evaluation of wide bandgap semiconductor materials.

Key words： SIMS， Wide bandgap semiconductor materials, SiC, GaN, SCM

Insights into chemical composition of turbocharger deposits using OrbiSIMS

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The buildup of insoluble deposits on key combustion engine parts which result in the wear of components and increased emissions is a growing issue that warrants investigation. Previous work by Edney et al. [1] analyzed deposits in pre-combustion fuel injectors by Orbital trapping secondary ion mass spectrometry (OrbiSIMS) depth profiling showcasing the utility of this approach to define their molecular chemistry and distribution. By applying molecular formula prediction (MFP) chemical filtering [2], key chemistries of the deposits such as inorganic salts and polycyclic aromatic hydrocarbons (PAHs) were discovered as multi-layered entities.

This investigation builds on previous engine deposit studies, however, focuses on turbochargers, now a widely applied technology in modern day exhaust systems which increase combustion efficiencies by taking advantage of the high energy internal combustion exhaust air. Samples of small sections from once operational fouled turbochargers were analyzed (Fig. 1a). OrbiSIMS analysis of these samples employing MFP [2] revealed a series of chemistries present such as PAHs $m/z > 800$, N-PAHs as well as calcium and sodium salts. (Fig. 1b). Of these chemistries, calcium salts were observed as being unique relative to previously studied engine deposits [1f]. It is believed that these originate from lubricating oil additives and their depth profile suggests that they are present throughout the bulk of the deposits and may contribute to their formation The turbocharger encounters combustion exhaust gas directly after expulsion from the chamber and therefore analysis of the carbon content of the deposits provides a chemical insight into the formation of soot and how the structure and ordering of carbon differs from that found in pre-combustion fuel injectors. This work enables an understanding of the currently unknown “inception” phase in soot development [3].

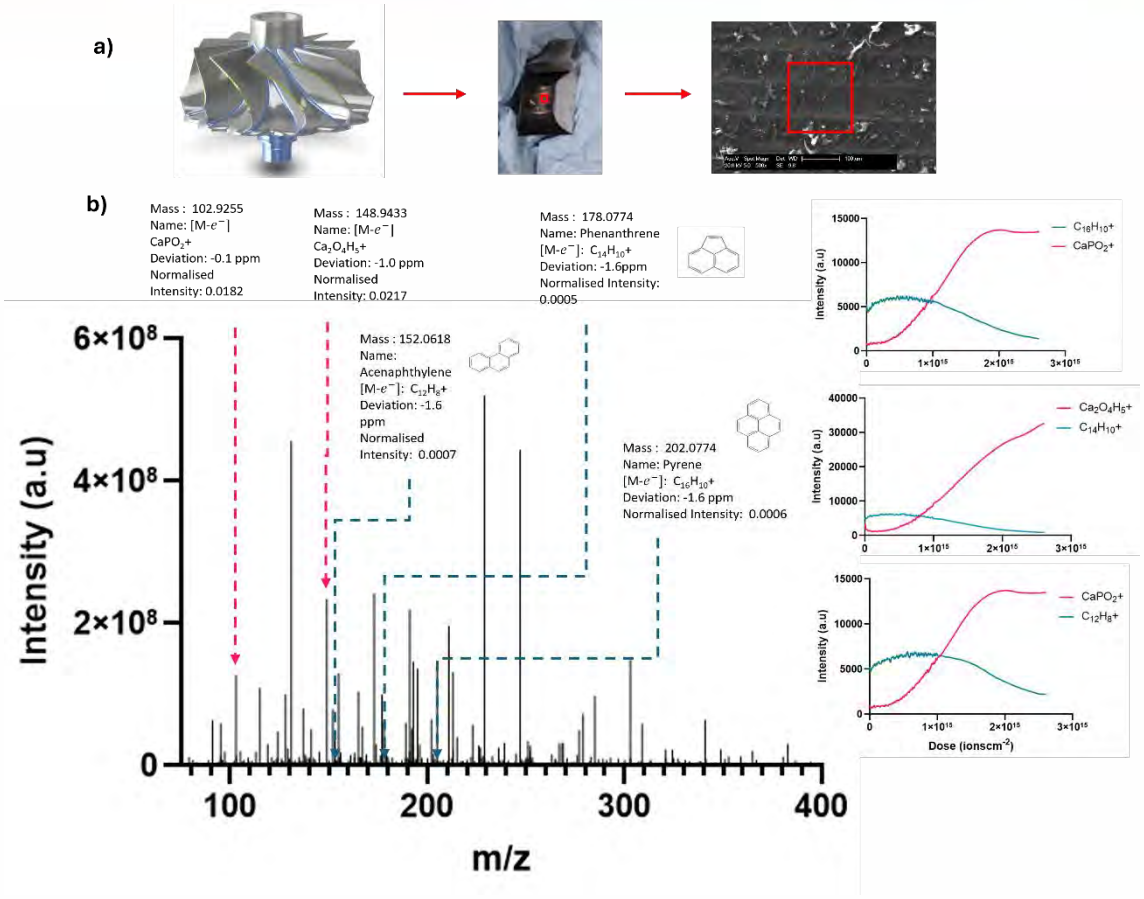


Figure 1: a) Right to left: Diagram of turbocharger turbine [4] , photo of fouled turbocharger sample, SEM image of the deposit surface b) OrbiSIMS spectra and corresponding depth profiles indicating key carbon and calcium molecular ion species in the surface and bulk layers).

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Therapeutic Drug Monitoring of Human Blood Samples by Using Nanosheet-Assisted LDI-TOF

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Therapeutic drug monitoring (TDM) demands rapid, sensitive, and clinically adaptable analytical platforms. Here, we present a nanosheet-assisted laser desorption/ionization time-of-flight mass spectrometry (LDI-TOF MS) strategy that enables direct, matrix-free detection of therapeutic drugs in human blood.

We first demonstrated that nanostructured inorganic surfaces can replace conventional organic matrices, enabling efficient ionization of small-molecule drugs with significantly reduced background interference and simplified sample preparation [1]. This work established the feasibility of nanomaterial-assisted LDI for bioanalytical applications.

Building on this foundation, we identified tellurium-containing transition metal dichalcogenide nanosheets ($MoTe_2$, WTe_2) as highly effective ionization platforms, achieving markedly enhanced sensitivity and multiplexed detection of antiepileptic drugs in human serum [2]. The method showed strong agreement with clinical gold standards (immunoassay and LC–MS/MS), demonstrating its translational potential for real patient samples.

To uncover the mechanistic origin of this enhancement, we elucidated interfacial charge-transfer dynamics using integrated experimental and theoretical approaches [3]. We revealed that photoinduced hydroxyl radicals, proton-coupled charge transfer, and surface electronic structure synergistically govern ionization efficiency. In particular, surface charge localization and conduction-band energetics were identified as key descriptors that drive Coulombic repulsion and facilitate efficient analyte desorption.

In summary, nanosheet-assisted LDI-TOF MS transforms TDM by eliminating conventional matrix limitations while achieving high sensitivity, rapid analysis, and clinical compatibility. By linking nanoscale electronic structure to macroscopic analytical performance, this approach provides a generalizable design framework for next-generation bioanalytical platforms and enables a practical pathway toward point-of-care diagnostics and precision medicine.

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Investigating changes to the glomerular filtration barrier in pregnancy and renal disease using ToF-SIMS

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Glycosaminoglycans (GAGs) are important biomolecules composed of repeating disaccharides that are associated with multiple biological processes. They have large structural heterogeneity associated with sulphation and deacetylation modifications that poses a significant analytical challenge. Time of flight secondary ion mass spectrometry (ToF-SIMS) is ideal for *in-situ*, label free GAG analysis [1] as it is capable of providing concurrent spatial and compositional analysis. To achieve this, GAG specific ions were identified based on their presence in the spectra of individual GAG standards and absence or appearance in GAG knock-out / knock-in cell lines. These ions were used to explore changes in GAG composition and spatial organisation in several pathologies through the analysis of tissue samples.

Alport syndrome (AS) is a rare inherited disease caused by mutations in collagen IV coding genes. It causes increases in proteinuria that becomes 10-fold exacerbated during pregnancy. Whole cross sections and individual glomeruli, the structure responsible for urine filtration, from murine renal tissue from healthy and AS pregnant and non-pregnant groups were analysed to investigate the role of GAG in this time specific change. The total ion intensity of the GAG chondroitin sulphate (CS) increased on a tissue wide and individual glomerular scale in healthy pregnancy only. We hypothesize that this is a compensatory mechanism present in healthy physiology which functions to minimize the impact of pregnancy on vascular integrity and that this mechanism is absent in AS which, when coupled to disrupted collagen in the basement membrane, leads to severely exacerbated proteinuria during pregnancy. Here SIMS analysis of kidney tissue enabled novel insights into the role of CS within AS without requirements for GAG labelling or labour-intensive GAG extraction.

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Pesticide analysis in Honeybee

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Increasing pressure on global food production can be partly addressed through the effective control of crop pests including through the application of pesticides. It is important to understand the adsorption, distribution, metabolism and excretion (ADME) characteristics of applied pesticides both in target pests and in other organisms including honeybees, to maximise effectiveness and minimize wider environmental impacts. Current analytical methods including autoradiography are extremely expensive, low throughput and do not give a complete description of pesticide metabolism and distribution. Here we present a methodology for mass spectrometry imaging of pesticide in honeybee (*Apis Mellifera*).

Honeybees were flash frozen in liquid nitrogen and stored at -80˚C before embedding in 2% (*w/v*) solution of sodium carboxymethylcellulose (CMC) solution in water and cryosectioned at -25 ˚C. Mass spectrometry imaging compatible tapes [1] were used for mounting whole-body cryosections onto suitable substrates. After freeze-drying samples were exposed to pesticide solutions. Imaging was performed with ToF-SIMS (J105, Ionoptika Ltd) and Desorption Electrospray Ionisation (DESI) (Xevo Q-ToF, Waters Corp.). We report on method development and choice of analytical conditions, comparing limits of detection and tissue-specific matrix effects. This proof of concept work demonstrates the analytical capabilities of mass spectrometry imaging in pesticide-insect studies.

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Observing the real-time effects of PRRT therapy on patients with neuroendocrine tumors by ToF-SIMS measurements of blood serum.

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Peptide Receptor Radionuclide Therapy (PRRT) is based on radiopharmaceutics, which binds preferably to overexpressed somatostatin receptors on neuroendocrine tumor cells, enabling precise administration of radiation. The course of treatment include 4 doses of drug every 8 weeks.As a lot of metabolites are transported with blood serum, changes in its chemical composition give a lot of information about body homeostasis and its abnormalities, including the reaction of cancer cells to oncological therapy.

To observe the effects of PRRT treatment on patients, samples of peripheral venous blood serum were collected at 9 time-points: before and 2 weeks after every administration of radiopharmaceutic, as well as 2-3 months after completion of treatment. Study was performed on 104 samples from 20 patients. Each sample was measured with ToF-SIMS in 5 randomly selected places on dried drop to account for inhomogeneities. The trends in samples were analyzed with Principal Component Analysis.

On Fig. 1. with PC3 of negative spectra, after each administration (samples 2, 4, 6, and 8), a transient drop was observed, followed by recovery. The peaks on positive loadings of PC3 were, among others, $C_{18}H_{33}O_2$-, $C_{18}H_{37}NO$- and $C_{16}H_{33}NO$-, and on negative loadings CH_3SN_2-, $C_9H_{17}O_2$- and $C_2H_4N_3$-. This trend suggested changes in metabolism and was most probably caused by decreasing of cancer burden after each administration, and the regrowth of disease before next one.

The results of this research suggests that studying the changes in composition of blood serum with the ToF-SIMS method can provide unique information about real-time reaction to therapy.

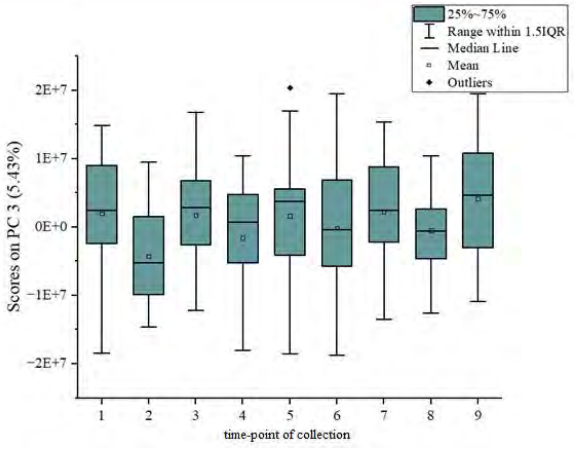


Fig. 1

Layer by Layer: Decoding Biosensor Surface Evolution via ToF-SIMS

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The rational design and fabrication of biosensors rely on the precise control of sequential surface modifications, each of which critically determines the final device sensitivity, specificity, and reproducibility. However, the conventional approach of validating a biosensor solely through its analytical response fails to provide molecular-level insight into the individual functionalization steps, leaving potential sources of failure, such as incomplete layer deposition, probe desorption, or incorrect antibody orientation, undetected until late in the development process [1]. Biosensor surface modifications involve different molecules, including specific binding molecules and blocking agents, accomplished following multi-step functionalization and assay procedures, but discrimination of these molecules is not provided by biosensor response alone. Case studies presented here span a broad range of biosensor platforms and target analytes, from gold substrates functionalized with thiol-modified self-assembled monolayers (SAMs) for protein biodetection, where ToF-SIMS proved useful for monitoring all functionalization steps including the biological behaviour of modified surfaces in the presence of target proteins. Recent developments of biosensors for inflammatory biomarker detection, including the application of QCM-based immunosensors functionalized with nanoparticle-coated surfaces for haptoglobin quantification as a neuroinflammation proxy, exemplify how layer-by-layer surface monitoring is becoming integral to next-generation device validation [2]. We used ToF-SIMS to validate the layer-by-layer assembly of a QCM immunosensor and electrochemical sensors for the inflammatory marker haptoglobin. Three sequential modifications: PEG-amine self-assembly monolayer SAM, hyaluronic acid-coated lipid nanoparticles (HA-SLNs), and anti-haptoglobin antibodies, were each characterized by their unique secondary ion fingerprints. ToF-SIMS confirmed successful SAM formation (e.g., CN^-, CNO^- ions), HA-SLN immobilization (enhanced carbohydrate-related fragments), and antibody coupling (characteristic amino acid-derived ions). Principal component analysis clearly discriminated each layer, revealing no cross-contamination or incomplete reactions. This molecular validation ensured that the final biosensor surface was chemically correct and reproducible, directly supporting its subsequent high-sensitivity detection of haptoglobin.

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ToF-SIMS imaging of immunolabelled neuroproteins

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Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) is a surface sensitive technique used to analyse different species including metals, small molecules and lipids [1]. However, higher molecular weight species such as proteins are not easily ionised and detected without fragmentation.

One way to image proteins using ToF-SIMS is through labelling them with lanthanide-conjugated antibodies [2]. We have been working on optimising this methodology and correlating it with immuno-based imaging approaches, e.g. immunofluorescence microscopy, to localise proteins such as glial fibrillary acidic proteins (GFAP) in tissue (Figure 1). We are developing this approach to be able to apply it to neurodegenerative diseases, such as familial amyotrophic lateral sclerosis (fALS). ToF-SIMS analysis of fALS mouse models may inform on pathological changes by enabling us to simultaneously identify the distribution of proteins along with the surrounding chemical environment made up of lipids, inorganic and small molecules.

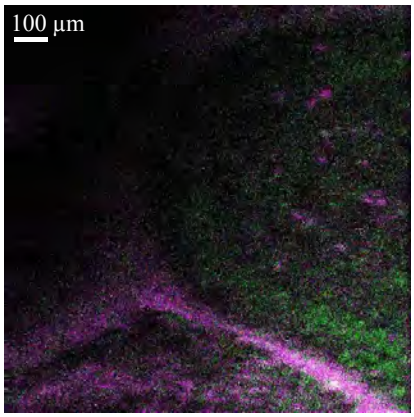


Figure 1. ToF-SIMS image (1200 × 1200µm) of mouse brain tissue. Iridium binding DNA (green), and lanthanide-conjugated antibodies labelling GFAP (purple).

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SIMS and XPS study of influence of the oxidizing technique on the biocompatible and corrosion properties of Ti6Al4V in a physiological environment

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We studied the corrosion and biocompatibility properties of oxide films generated on Ti6Al4V alloys using both traditional and novel methods. Oxide films were generated by anodization and plasma treatment to achieve a blue surface finish [1]. The oxide films were then characterized and compared to a native film formed on the Ti6Al4V. Electrochemical tests, incorporating potentiodynamic tests and electrochemical impedance spectroscopy, were employed to define the electrochemical resistance of oxides in an environment simulating biological exposure. In vitro tests were conducted to study ion release and biocompatible properties over a 6-week period of exposure to a 0.9 wt% NaCl solution, at body temperature. Various spectroscopic techniques, including ToF-SIMS, XRD, and Raman analysis, were used to study the structure and chemistry of the oxide films. The sub-surface layer was analysed by microstructural investigation. ToF-SIMS and XPS depth profiling of thin oxidized films before and after ion released measurements showed different presence of V in surface layer for different oxidizing methods.

It was found that the type of oxidation has a key influence on the composition of an oxide, especially with respect to the cross-sectional distribution of the oxides of the individual alloying elements across the oxide film. The type of oxidation was found to have a key influence on the oxide composition, especially with respect to the cross-sectional distribution of the individual alloy elements through the oxide film. The oxidation process determines which of the alloying elements are released into the environment, as a result of the corrosion reactions.

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Elucidation of Molecular Turnover in Neural Stem Cells using SIMS: Insights into Schinzel-Giedion Syndrome and RNA Therapy

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Biological molecules exhibit distinct cellular localizations that are closely linked to their functions. Molecular turnover, in which damaged cellular lipids and proteins are gradually replaced to maintain a healthy proteome and lipidome, plays a key role in stem cell behavior and functionality. Disruptions in this process can affect the regulation of stem cell fate, leading to disease and degeneration. Secondary ion mass spectrometry (SIMS), with its high sensitivity, versatility, and spatial resolution, has been increasingly applied in neuroscience, allowing the visualization of molecular localization and turnover at single cell and subcellular resolution. Here, we employed ToF-SIMS and NanoSIMS imaging to investigate lipid and protein turnover in neural stem cells, with a focus on differences between healthy and Schinzel-Giedion Syndrome (SGS) conditions, and the effects of a therapeutic intervention using antisen oligonucleotide (ASO).

ToF-SIMS was used to investigate membrane lipid composition and turnover in oligodendrocytes from healthy and SGS models, revealing disease-associated alterations in lipid accumulation and dynamic changes. On the other hand, correlative NanoSIMS imaging with electron microscopy enabled the characterisation of protein turnover at individual organelles of nerve cells.

The results showed that SGS results in significant alterations in both lipid and protein turnover. Notably, the ASO treatment partially restores these turnovers toward a healthy state, indicating recovery of cellular homeostasis at the molecular level. The work highlights the capability of SIMS imaging to connect molecular turnover with cellular function and disease, providing insight into neural stem cell regulation and therapeutic response in SGS.

Multimodal Correlative Imaging for Nucleic acid therapeutics

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Mapping the subcellular partitioning and intracellular trafficking of nucleic acid therapeutics (NATs) is fundamentally critical for understanding their complex mechanisms of action, evaluating off-target effects, and ultimately optimizing their clinical efficacy. While Nanoscale Secondary Ion Mass Spectrometry (NanoSIMS) enables high-resolution chemical imaging of labeled therapeutics, interpreting these sparse signals requires precise correlation with electron microscopy (EM) to place them properly within their cellular ultrastructural context. Because this correlative process is traditionally performed manually, making it highly labor-intensive and operator-dependent, we present a novel, automated multimodal imaging platform tailored for mapping NATs at multiscale and organelle-level resolution in both cells and tissues. To systematically visualize NAT behavior, we engineered an orthogonal labeling strategy incorporating nuclease-stable halogenated nucleotides. This approach allows distinct therapeutic components to be uniquely labeled with specific isotopes, enabling simultaneous, high-resolution NanoSIMS tracking. To achieve seamless cross-scale alignment across large EM datasets, we developed a computational pipeline that strategically leverages morphology-rich ion channels to robustly align molecule-specific, low signal-to-noise therapeutic channels directly with ultrastructural maps. Applying this comprehensive framework in vitro and in vivo revealed critical insights into NAT subcellular distribution. We observed that NATs primarily accumulate in endolysosomes, exhibiting highly heterogeneous signal intensities that indicate dynamic intracellular processing and partial structural dissociation within the cytoplasm. Furthermore, these therapeutics displayed complex localizations across distinct nuclear and cytoplasmic microenvironments, suggesting dynamic trafficking pathways beyond canonical mechanisms. Ultimately, this generalizable platform successfully bridges chemical and ultrastructural imaging modalities, overcoming therapeutic signal sparsity to provide a streamlined framework for subcellular pharmacology,

Key words: NanoSIMS, nucleic acid therapeutics

Investigating and characterising glycosaminoglycans within the cancer matrix

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Glycosaminoglycans (GAGs) are polyanionic, linear polysaccharide chains composed of repeating disaccharide units of an amino sugar and a uronic acid. Except hyaluronic acid, GAGs are located on the cell surface and in the extracellular matrix (ECM), covalently bound to protein cores. They form proteoglycans that are expressed ubiquitously throughout mammalian tissues and are essential in regulating cell signalling and tissue organisation[2]. Due to their abundance and functional versatility, GAG dysregulation is a known driver of multiple disorders, including tumour invasion, progression and metastasis. However, the mechanisms through which GAGs affect disease remain poorly understood, constrained by the technical limitations to assess their molecular distributions due to their structural heterogeneity, structural isomerism and variable molecular weight [1,2].

In this study, we aim to leverage the high spatial-resolution capabilities of the Time-of-flight (ToF) Secondary Ion Mass Spectrometry (SIMS) to provide *in-situ* compositional information of GAG distributions [3] in breast and ovarian cancer tumour cores and tumour-deposited ECM. In solid tumours, we integrated multiplex immunofluorescence with ToF-SIMS to colocalise the cellular phenotypic information with GAG ion intensity. Fluorescence markers were used to first identify regions of interest, such as tumour and stromal regions within the same core, which could be used to extract region-specific assessments of GAG composition. We then examined GAG ion intensity differences across malignant and non-malignant ECM models exposed to macrophages to characterise immune-mediated ECM remodelling, linking localised ion signatures to functional GAG presence within the tumour microenvironment.

Defining these molecular changes offers the potential to uncover novel biomarkers and therapeutic targets within tumour tissues.

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In Situ Variable-Temperature Liquid SIMS for Subzero Analysis

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In situ liquid time-of-flight secondary ion mass spectrometry (SIMS) technique has been invented by interfacing vacuum-based SIMS with a homemade microfluidic device of high vacuum compatibility for more than a decade, and significantly advanced with universal applicability through the utilization of the poly (ether ether ketone) (PEEK) block exhibiting exceptional chemical stability. Due to the widely demonstrated soft ionization feature, *in situ* liquid SIMS allows precise molecular discrimination of various microstructures such as ion solvation structures within both aqueous and non-aqueous liquids. Moreover, in comparison with traditional mass spectrometric tools, e.g. electrospray ionization (ESI)-MS, *in situ* liquid SIMS can directly analyze a wide range of liquid samples, even those with highly concentrated salts and/or air-sensitive liquids, without need of any sample pretreatment, which enables the detection of molecular structures of liquids in their original status. However, currently *in situ* liquid SIMS can only deal with liquid samples at room temperature.

Recently, we developed an advanced *in situ* variable-temperature liquid SIMS technique by interfacing in situ liquid SIMS with a thermal-conductive copper (Cu)-based microfluidic device that is attached on a temperature-controllable sample stage. Utilizing *in situ* variable-temperature liquid SIMS, we for the first time accessed the direct molecular evidences to discriminate the corresponding evolution of complex ion solvation structures and water structures in the subzero water-in-salt electrolyte, which may not be feasible for ESI-MS. This work opens a new avenue for bridging the gap in the knowledge of the correlations between the microscopic structures and macroscopic properties of subzero electrolytes.

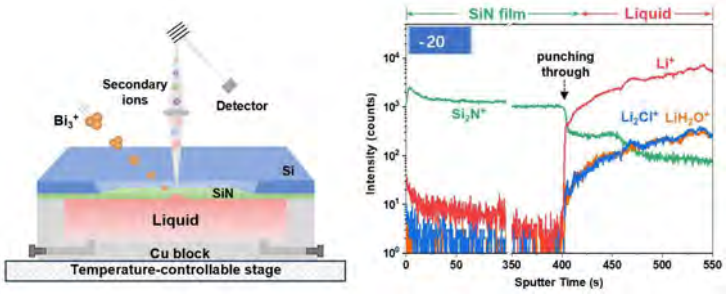


Figure 1. In Situ Variable-Temperature Liquid SIMS.

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Advanced Interfacial Analysis of Composite Polymer Electrolytes – High Resolution ToF-SIMS Imaging combined with Orbitrap-SIMS

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The development of next-generation batteries critically depends on a detailed understanding of interfacial chemistry and ion transport in advanced materials. Composite polymer electrolytes (CPEs), which combine inorganic fillers with polymer matrices, exhibit promising mechanical and physicochemical properties for such applications. However, characterizing them remains challenging due to the sensitivity of the polymer matrix, which complicates interfacial analysis.[1]

In this study, we present an advanced analytical workflow that integrates high-resolution secondary ion mass spectrometry (SIMS) imaging, offering both high lateral and mass resolution, with electrochemical characterization of CPEs. CPE samples were prepared using inorganic fillers with different surface treatments. Cross-sections were obtained via cryogenic ion beam milling to preserve structural integrity.

Subsequent Time-of-Flight SIMS (ToF-SIMS) imaging with delayed extraction enabled precise spatial localization of signals associated with the surface treatments at the interfaces between inorganic particles and the polymer matrix. To confidently assign molecules in the higher mass range, Orbitrap-SIMS was employed, achieving a mass resolution of up to R = 240,000. The resulting chemical information was then correlated with the electrochemical performance of the investigated CPEs.

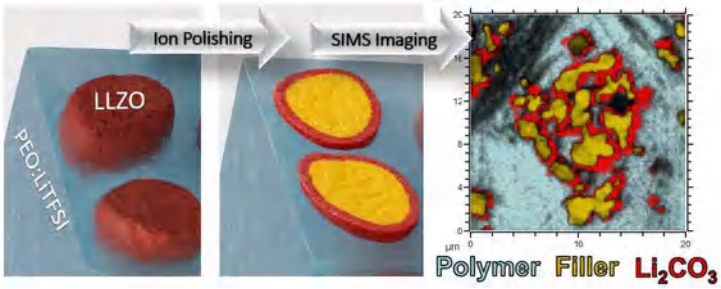


Figure 1: Schematic of cross-section preparation and ToF-SIMS Imaging of CPE cross-section showing interfacial $Li_3CO_3^+$ signal around LLZO particles after air treatment.

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Optimising Depth Analysis for Complex Semiconductor Materials: Using Small Cluster size of Ar Cluster SIMS at High Beam Energy Under Cryogenic Conditions

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Gas cluster ion beams (GCIBs) are predominantly considered as a low-damaging sputtering technique for surface analysis of organic and biological samples. For example, ionised clusters of atoms/molecules accelerated to high energies (keV) are highly efficient at sputtering intact molecules from surfaces in SIMS experiments with less damage than monoatomic beams. However, GCIBs are highly versatile having variable beam energy ranges and utilising a range of gas species; large GCIB (large cluster beam) for sputtering of high mass molecules and small GCIB (small cluster, high energy beam) for reducing intermixing and preferential sputtering effects on hard and soft mixed materials.

The current common approach to analyse hard and soft mixed materials such as perovskite solar cells is to peel off the hardest capping layer and then analyse the perovskite layers using Ar GCIB to sputter and Bi to analyse using ToF SIMS. Alternatively, a Cs beam may be used to sputter to just above the interface, and then low energy an Ar GCIB and Bi beam used for sputtering and analysis. However, these approaches are flawed; the peeling process can cause migration of elements to the free surface, and Cs and monoatomic Ar sputtering can cause intermixing of consecutive layers. We have previously demonstrated use of smaller cluster beams to sputter though 1.5 um thickness of perovskite solar cell samples from the capping layer to the glass substrate with less preferential sputtering and intermixing effects. In addition, the Ar GCIB is used not only for sputtering but also analysing in our unique J Series III Cluster SIMS (Ionoptika Ltd.), therefore, the data can show how the components chemically reacted in the material as 3D images. Depth analysis using a small cluster GCIB in our Cluster SIMS system promises to show more 'genuine' information than the current dual beam method for hard and mixed materials including metals and organics.[1]

SIMS may be performed at cryogenic temperatures. However, complex cryogenic sample handling requirements and high cryogen consumption have meant that such experiments have hitherto been expensive and complicated. In this work, we demonstrate the suitability and lack of preferential sputtering using small Ar GCIBs at a high beam energy (70 keV) for semiconductor materials such as perovskite solar cells and show that the precision of the depth profile is increased at Cryo temperatures when compared with RT analysis.

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SIMS Across Timescales: Three Perspectives on Battery Interfacial Chemistry

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Understanding battery interfaces requires analytical tools that can capture chemical processes across vastly different timescales, from the earliest stages of interface formation and transient reaction intermediates to cumulative degradation over hundreds of cycles. This talk presents secondary ion mass spectrometry (SIMS) as a versatile platform for addressing this challenge. Three complementary perspectives from ongoing work in our group are used to illustrate this.

Firstly, we demonstrate how in situ SIMS allows the controlled investigation of solid electrolyte interphase (SEI) formation, providing chemical insight into the initial stages of interfacial development.[1] Secondly, operando SIMS demonstrates its unique ability to detect transient species in real time, as demonstrated by the observation of redox-active iodine intermediates during electrochemical cycling, a class of information that is largely inaccessible by other analytical methods. Thirdly, post-mortem analysis of cathode active materials shows how high-resolution SIMS captures the cumulative fingerprint of interfacial reactions in the cathode-electrolyte interface (CEI), linking cycle history to composition and electrochemical performance.[2]

Together, these examples demonstrate the unique contributions of SIMS to the study of battery interfaces, including its ability to bridge timescales, complement established electrochemical and analytical methods, and reveal mechanistic details that would otherwise remain hidden.

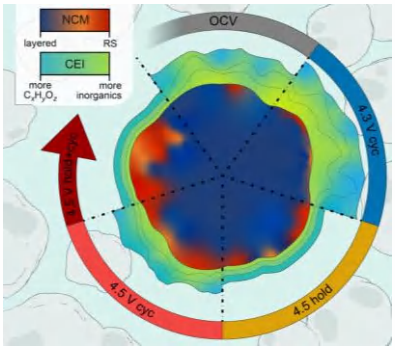


Figure 1: Post-mortem SIMS analysis of the CEI on NCM: schematic summary of the dependence of CEI composition on upper cutoff voltage and cycling protocol.[2]

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An Argon Gas Cluster Ion Beam (GCIB) based ToF-SIMS approach for Ultra-Trace Lithium Profiling in microelectronic materials

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Accurate localization of trace alkali contaminants in dielectric materials is analytically challenging, yet necessary to guide the integration of alkali rich materials (e.g. solid state microbatteries for chip power integration) in microelectronic devices. Lithium is of particular concern, because even at very low concentration it can migrate under electric field or diffuse at relatively high temperature, thereby altering oxide growth processes [1] and possibly degrading device performance. Over the last decades, ToF-SIMS has been established as one of the most relevant techniques for trace alkali analysis because of its high sensitivity and its localization capability. However, reliable lithium quantification and localization remains challenging due to limitations such as beam-induced ion migration [2].

In literature, most currently available approaches for lithium depth profiling are either time consuming (e.g. cryogenic conditions) or lack sensitivity, and therefore remain inapplicable to ultratrace analysis (ppm-ppb). While conventional O_2^+ sputtering is commonly used to enhance positive secondary ion yields, it can also induce surface charging and ion beam induced migration [3]. However, although GCIB has been extensively applied to organic materials, its use in the study of inorganic materials remains underexplored, and only limited literature is available on their application to lithium and other alkali metal profiling [4].

In this context, we developed an Ar-GCIB-based protocol for the analysis of ultra-traces of lithium in Si and SiO_2 (down to 10^{12} at/cm^{-2}). ^{7}Li implanted silicon oxides layers were analysed under these optimized sputtering conditions.

We show that, compared with conventional O_2^+ sputtering, our optimized protocol provides an effective strategy to mitigate beam-induced artefacts and improve the reliability of ultra-trace lithium depth profiling.

In addition, Li diffusion kinetics were investigated *in situ* over a temperature range commonly used in microelectronic processing.

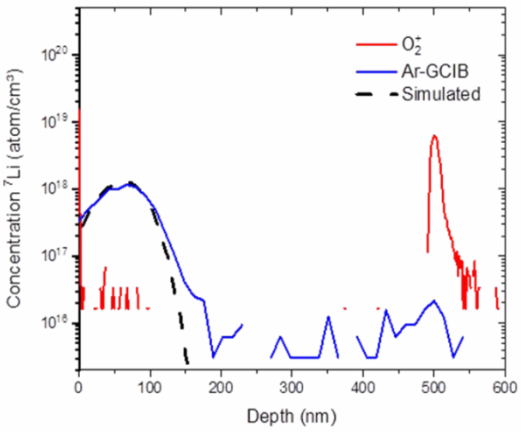


Figure : Comparison of ToF-SIMS depth profiles of Lithium in thermally grown silicon oxide using different sputter ion species

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Acknowledgements
This work, carried out on the Platform for Nanocharacterisation (PFNC), was supported by the "Recherche Technologique de Base" and "France 2030 - ANR-22-PEEL-0014" programs of the French National Research Agency (ANR)

Refining experimental conditions for accurate SIMS characterisation of abrupt interfaces in III-V semiconductors

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III-V materials (arsenides & phosphides) are interesting for the fabrication of high-frequency transistors and semiconductor lasers, which are essential for current communication challenges (6G telecommunications, optical communications, lidar, etc.). In the context of devices fabrication, it is crucial to control the abruptness of interfaces in $In_{(1-x)}Ga_xAs$ / InP heterostructures.

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) and magnetic sector secondary ion mass spectrometry (SIMS) have proved ideal for studying these buried interfaces [1,2]. However, the analysis may be impeded by ion-beam mixing of Ga near the interfaces and possibly by preferential sputtering of As or P. For III-V semiconductors, the choice of abrasion conditions is therefore decisive to obtain reliable depth profiles.

In this work, we study the influence of various parameters such as the energy or the incidence angle of the primary ion beam, sample rotation or temperature.

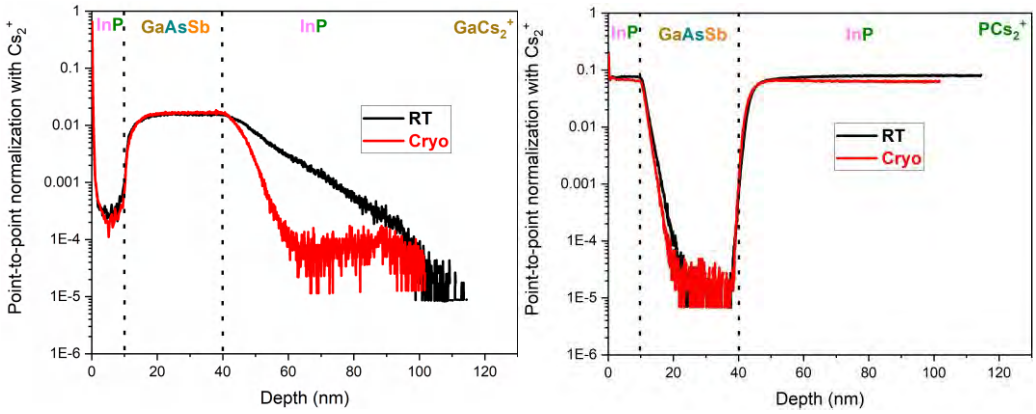


Figure 1. Overlay of positive polarity ToF-SIMS depth profiles acquired at room temperature (black) and under cryogenic conditions (red) respectively for $GaCs_2^+$ (left) and PCs_2^+ (right) [3].

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Acknowledgement
This work, carried out (in part) on the Plate-Forme de Nano-Caractérisation (PFNC), benefited from government funding managed by the Agence Nationale de la Recherche under the "Recherche Technologique de Base" and France 2030 programs (ANR-22-PEEL-0014). We would also like to thank the Labex MINOS (ANR-10-LABX-0055) for funding this project.

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Is this atom single?

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Noble metal co-catalysts can significantly enhance the catalytic performance of semiconducting materials. The trend towards highest possible activity combined with the lowest possible amount of the expensive and rare co-catalyst led to the development of the research field of single atom catalysis. A strong enhancement of activity is typically observed for well-distributed co-catalyst in the single-atom state, while clustering of the co-catalysts often show a drop in efficiency.[1] In recent publications, the entire enhancement of catalysis was attributed to co-catalysts in the single atom state instead of nanoparticles.[2] Analysis of single atoms bound to a semiconductor surface, however, typically requires proof by high-angle annular dark-field transmission electron microscopy (HAADF-TEM) or electron paramagnetic resonance (EPR) spectroscopy, both of which are expensive and often not readily accessible techniques. We were the first group to demonstrate a difference in fragmentation caused by single atoms of Pt immobilized on TiO_2 compared to Pt clusters in ToF-SIMS.[3] Single atom state Pt was shown to produce clear PtO_x^- signals, most likely originating from Pt bound to the oxide surface. We extended the analysis of co-catalysts immobilized on an oxidic support (e.g., TiO_2, NiO, ZrO_2) to further co-catalysts of interest, e.g., Cu, IrO_2, V_2O_5, and analyzed differences in the spectral pattern in dependence of the co-catalyst amount.

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ToF-SIMS Investigation of Adsorption and Desorption Processes in Sur-MOF Thin Films for Environmental Water Remediation

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The increasing release of persistent organic contaminants from industrial activities, particularly textile dye effluents, demands advanced materials for efficient water remediation. In this context, Surface-supported Metal–Organic Frameworks (Sur-MOF) have emerged as promising systems due to their high porosity and tunable structure.
In this work, Cu-BTC (copper–benzene-1,3,5-tricarboxylate) Sur-MOF thin films were synthesized via a wet Layer-by-Layer (LbL) deposition method on quartz substrates, previously functionalized with a zirconium phosphate-phosphonate interlayer to ensure controlled growth and stable anchoring. The adsorption performance of the films was evaluated using Rhodamine B as a model dye pollutant and regeneration experiments were performed to assess reusability.
Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) was employed as a key technique to obtain detailed mass spectra, enabling the identification of characteristic fragments of both the Cu-BTC framework and the adsorbed dye, thus confirming successful pollutant uptake. UV–Vis spectroscopy and Atomic Force Microscopy (AFM) were used as complementary techniques to correlate optical response and surface morphology.
The results demonstrate the effectiveness of Cu-BTC in capturing organic pollutants and confirm their potential as versatile and reusable materials for advanced water remediation applications. Notably, ToF-SIMS technique enables direct molecular-level monitoring of both absorption and desorption, offering unique insight into the dynamic surface chemistry of Sur-MOF systems.

Acknowledgments: This work was partially supported by the European Union's Horizon Europe research and innovation programme under the EIC Pathfinder Open project ERMES – Information Transfer Between Medical Doctors and Implanted Medical Devices via Artificial Molecular Communication (Grant Agreement No. 101185661).

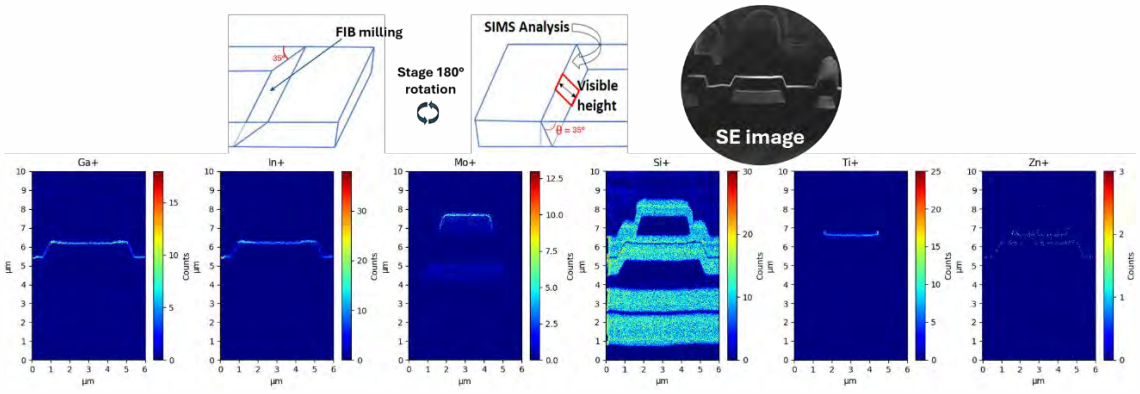
Multi-Modal FIB-ToF Methodologies to Address Nanoscale Characterization Challenge in Microelectronics

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(1) *Tescan France, Fuveau, France*
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The rapid development of advanced materials, particularly in microelectronics, increasingly demands ultra-high-resolution analytical tools capable of probing chemical, structural, and compositional properties at the nanoscale. Traditional characterization techniques often fall short in providing comprehensive, multi-scale insights required to understand and optimize these complex systems. To address this need, we leverage the NanoSpace platform (Orsay Physics), a versatile UHV modular system that integrates a wide range of analytical techniques, including Focused Ion Beam (FIB), Scanning Electron Microscopy (SEM), Gas Injection System (GIS), Orthogonal Time-of-Flight Secondary Ion Mass Spectrometry (O-TOF-SIMS), and also EDX and EBSD. Its modularity and extensive configuration options, including a broad selection of ion sources, enable tailored solutions for diverse applications, from dopant mapping to interface analysis and 3D chemical imaging [1,2].

In this work, we demonstrate how multiple ion source technologies and advanced methodologies within the NanoSpace platform were employed to tackle a challenging microelectronics application. By combining FIB, SEM, and O-TOF-SIMS, we achieved high-precision chemical and structural analysis, addressing critical questions such as pollutant distribution, and heterogeneity in 3D device at nanoscale.



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Cluster-induced desorption/ionization mass spectrometry of dye molecules – from fundamentals to OLEDs and forensic applications

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Dyes are ubiquitous in our daily lives and used in many industrial applications. The analysis of dyes is thus of relevance from various viewpoints, ranging from quality control in organic electronics over applications in life sciences to forensic investigations. In dye analysis, e.g., of written ink, desorption-based mass spectrometry methods have been shown as most powerful tools. Here we report on the application of desorption/ionization induced by neutral SO_2 clusters (DINeC) for the fragmentation-free desorption and unambiguous identification of the dye molecules and their degradation processes by means of mass spectrometry (MS).

As a prerequisite for the application of DINeC-MS to the wide variety of dye molecules, cationic, neutral, and anionic dyes were investigated with respect to their ionization/ desorption behavior [1]. All dyes, including fragile complexes such as the electroluminescent $Ir(ppy)_3$ which is used in OLEDs, were desorbed as intact molecular ions without fragmentation, but the ionization process strongly depends on the type of dye. E.g., cationic dyes are exclusively detected as cations without counterion whereas anionic dyes were detected both as anions and cations, e.g., with two of the counterions attached to the molecular dye ion. Furthermore, for $Ir(ppy)_3$, the ionization process was shown to strongly depend on the content of H_2O on/in the sample (Fig. 1, right). Application of the soft desorption technique in terms of studying/differentiating fragmentation processes induced by different stimuli, such as UV light, heat, or operational conditions, is demonstrated. It is based on (slight) differences in the fragmentation patterns which are only accessible to a fragmentation-free analysis method. (Fig. 1, left).

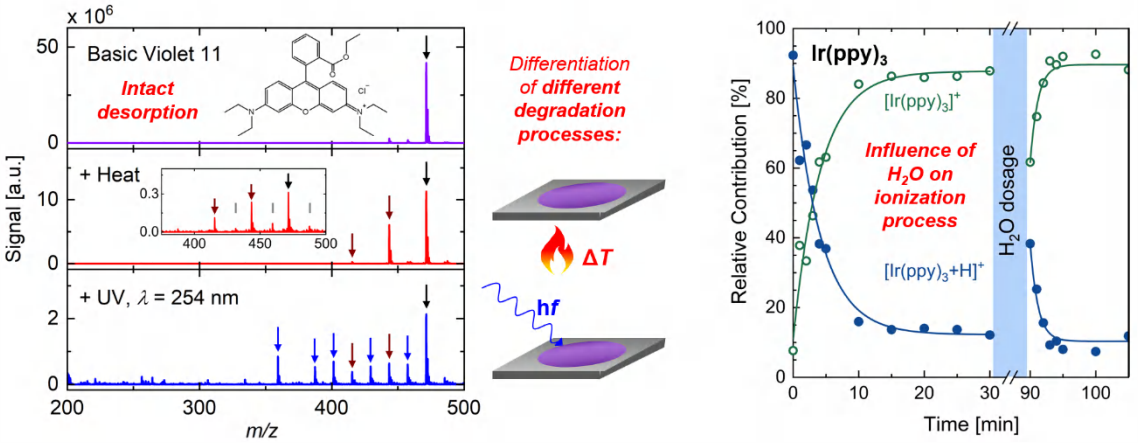


Fig. 1: Left: Intact desorption of basic violett and different fragmentation patterns induced by different stimuli. Right: Dependence of ionization process of OLED compound $Ir(ppy)_3$ on H_2O supply.

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Molecular Insights and Origins of Internal Combustion Engine Deposits via OrbiSIMS

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Instrument development in secondary ion mass spectrometry (SIMS) continues to yield more and more complex hyperspectral data-sets. These data-sets enable significant advancements in applications and research opportunities, however, they also possess an associated series of challenges to interpret them and unlock their full potential. This is exemplified in the introduction of Orbitrap SIMS (OrbiSIMS), where typical data-sets exhibit a 100 - 1000 fold increase in the number of secondary ions observed for any given sample as compared to comparable time of flight (ToF) data. As a materials analysis capability this has significantly impacted a multidisciplinary scope of academic and commercially focussed research areas from biology (e.g. in molecular analysis [1], cells [2] and tissues [3]) to engineering (e.g. 3D printing [4] and fuel deposit analysis [5]).

Carbonaceous fuel deposits are ubiquitous, being formed on surfaces in engines, fuel systems and on catalystsoperating at high temperatures for hydrocarbon transformations. In internal combustion engines, theirformation negatively affects worldwide vehicle emissions and fuel economy. Deposit composition and formation pathways are poorly understood due totheir insolubility and the intrinsic complexity of their layered carbonaceous matrix. Here, we apply OrbiSIMS to undersatand deposit chemistry and evidence common molecular distributions in deposit depth and in positions relative to the combustion chamber. We observe the productsof the growth of both planar and curved polycyclic aromatic hydrocarbons to form small fullerenes overtime in the engine and propose possible formation pathways which explain the molecular distributionsobserved. For the first time, OrbiSIMSresults were compared and validated with data from atmospheric pressure matrix assisted laser desorptionionization MS. The comprehensive characterization provided will help the development of a new generation of chemical additives to reduce deposits, and thus improve vehicle emissions and global air quality.

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Key words: OrbiSIMS, fuel deposits, polycyclic aromatic hydrocarbons

Characterization and Regulation of Local Chemical Orderings in High-Entropy Alloys via 3D Atom Probe Tomography

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With the increase of configurational entropy, the chemical complexity of materials gradually rises. The design philosophy of high entropy alloys (HEAs), based on the concept of entropy, has emerged as a promising approach to achieving the synergistic enhancement of mechanical properties such as strength and ductility. However, the complex atomic environment in these alloys makes the formation mechanisms of sub-microscopic or atomic-scale local structures and their influence on mechanical properties still unclear. This study focuses on three representative systems: high entropy disordered alloys, Nb-based nanocrystalline alloys, and high entropy MAX phase alloys. By integrating three-dimensional atom probe tomography (3D-APT) with advanced transmission electron microscopy (TEM), we investigate the formation and evolution of local chemical ordering (LCO) in different alloy systems. Starting from the atomic scale, we systematically explore the formation mechanisms, thermodynamic origins, and the role of LCOs in regulating defect evolution. Furthermore, we reveal the cross-scaled correlation between LCOs and mechanical properties. This report provides an in-depth analysis and summarizes effective strategies for tailoring atomic-scale structures in various alloy systems, offering new insights into the design of high-performance materials through local-ordering engineering.

Hybrid Methodologies for Interface Abruptness Analysis in Si/SiGe/Si Heterostructures

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Research on Si/SiGe heterostructures is paramount for the advancement of semiconductor devices, with interface interdiffusion posing a critical challenge that significantly impacts device performance. This study employs a hybrid methodology, integrating Atom Probe Tomography (APT), Transmission Electron Microscope (TEM), and Secondary Ion Mass Spectrometry (SIMS), to analyze interface abruptness in Si/SiGe/Si structures. A Si-capped 10 nm SiGe layer (33% Ge) epitaxially grown on a Si substrate was investigated. Following thermal annealing at 900°C for 10 minutes, significant Ge diffusion from the SiGe layer into the Si substrate was observed. The consistent results obtained from APT/TEM/SIMS analyses unequivocally confirm the extent of this interdiffusion. Furthermore, within the APT results, detailed discussions on local field effects, atomic density variations, and interface reconstruction issues were discussed, providing a clearer model for the result.

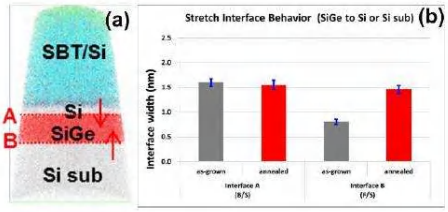


Figure 1. Figure 1 (a) shows an APT reconstruction with Si cap on SiGe/Si substrate. 1 (b) shows an interface diffusion defined by Ge iso-surface.

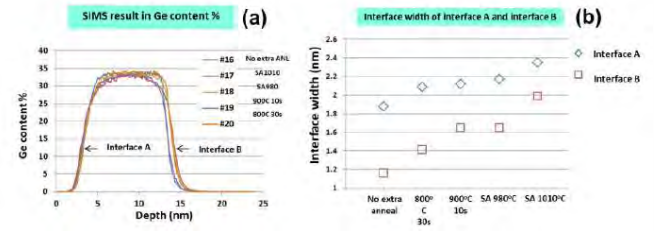


Figure 2. Figure 2 (a) shows a SIMS profile on same sample with APT. 1 (b) shows an interface diffusion defined by profile.

Toward Comparable Atom Probe Tomography: Reporting, terminology and a coordinated path forward

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Atom probe tomography has matured from a specialist technique into a routine analytical tool across semiconductors, batteries, structural metals, catalysis, and hydrogen-affected materials. With that maturity comes a quieter problem: reporting practice has not kept pace with the spread of the method, and results remain difficult to compare across laboratories even for well-studied systems. As atom probe data move into industrial qualification and failure analysis, inter-laboratory comparability is no longer only an academic concern.

This talk frames the issue and outlines how the international APT community has organized its response. Within IFES and ISO/TC 201/SC 6, work has proceeded on two fronts: a terminology effort building ISO-style definitions cluster by cluster, and a reporting effort grounded in an international survey of the user base. The survey drew a strong response and confirmed broad convergence on what should be reported; a community guideline paper based on those results is now in preparation. The practical stakes of the terminology work are illustrated through a concrete case, the definition of ion-beam diameter, where a small wording choice carries measurable consequences for how laboratories compare instruments.

The talk then maps how durable progress is most likely achieved: through coordination among the established bodies, with terminology and standards developing through ISO and inter-laboratory validation through dedicated metrology frameworks. Equally important is the domestic picture. China has its own active APT community, which has largely developed in parallel with the international effort. The most productive path is not to treat one as downstream of the other but to connect them, so that a domestically grounded effort, rooted in local priorities and capability, both informs and draws on the wider process. Speaking from a position within both communities, the talk closes with directions worth pursuing rather than fixed plans, and an invitation for the Chinese APT community to help shape a shared agenda.

Deciphering the single Neuronal Death Narrative: Sub-Micron Spatial Omics via water Cluster/C60 /Plasma SIMS

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Mapping the precise molecular cascades in individual cells that govern neuronal death is critical to uncovering the mechanisms and progression of neurodegeneration. However, mapping these intricate biochemical shifts has long been hindered by the trade-off between spatial resolution and single-cell molecular identification. Furthermore, the critical need to preserve pristine chemical gradients is frequently unmet, as these transient signals are typically lost during conventional sample preparation without a dedicated cryogenic workflow.

We present an advanced secondary ion mass spectrometry (SIMS) approach engineered to decode the spatial omic narrative of single deteriorating neurons. By leveraging multiple primary ion beams—specifically water cluster (H2O)n+n≥28,000), C60+, and focused Xe+ plasma beam—in tandem with a specialized cryogenic workflow to preserve volatile and transient biomolecules, unprecedented micron to sub-micron lateral resolution was achieved. This configuration enhances molecular ion detection of metabolites, lipids, and peptides in cells/tissues while simultaneously accommodating antibody-based cell-identity detection in a single sample. To process these multi-modal datasets, algorithms were developed to segment single cells, co-register cell death hallmarks to identified cells, and perform advanced spatial clustering analysis. The detection of low-abundance cell-death hallmarks was validated via Cryo-3D imaging of single HT22 cells, a mouse hippocampal neuronal line.

The workflow allowed for the simultaneous interrogation of endogenous omics profiles across different cell types without losing spatial context in tissues affected by traumatic brain injury (TBI). The co-optimized analytical and computational workflow successfully mapped localized biochemical transitions and resolved cellular boundaries. The downstream segmentation and clustering algorithms accurately isolated single-cell data, linking specific metabolic and lipidomic shifts to phenotypic hallmarks of ferroptotic death.

These findings demonstrate that high-resolution cluster/plasma SIMS successfully bridges the gap between ultrastructural imaging and untargeted spatial metabolomics. By capturing the final molecular signatures of individual neurons and mapping cellular crosstalk during neural decay, this methodology offers a rare opportunity to dissect neurodegenerative pathways and evaluate targeted neuroprotective therapeutics.

Key words: Cryo-SIMS, Sub-micron Spatial Omics, Single-Cell Analysis, and Ferroptosis

The Role of Lipids and Proteins in the Foreign Body Response at the Surface of Medical Implants

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Medical implants play a vital role in patient recovery, rehabilitation, and quality of life. In orthopaedic settings, they are widely used for fracture fixation, limb deformity correction, limb lengthening, and joint replacement. Devices such as screws, pins, wires, and plates are integral to these interventions, with ongoing innovation in implant design and biomaterials continuing to improve clinical outcomes. Successful fracture healing and implant integration depend on biological processes influenced by interactions between the implant surface and surrounding host tissue. However, the body may mount an adverse immune reaction known as the foreign body response (FBR). This complex process can lead to pain, inflammation, infection, fibrotic encapsulation, implant loosening, or rejection, potentially compromising device function and necessitating surgical explantation or revision. Managing the FBR therefore, remains a major challenge in biomaterials science and orthopaedic medicine.

Proteins have long been studied for their role in modulating the FBR, but emerging evidence now highlights the critical contribution of lipids at the biomaterial interface. Lipids are potent immunological mediators capable of influencing inflammation and fibrosis, yet their role in implant-associated immune responses remains underexplored. Recent work has shown that specific lipid species adsorbed onto implant surfaces can significantly influence immune activation and fibrotic responses, shifting current understanding of biomaterial-host interactions. Using Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), lipid-specific deposition patterns were shown to correlate with FBR severity in murine and human models [1].

The FIBRIS Study is building on this breakthrough by examining explanted orthopaedic pins and associated tissue samples from patients treated with the Taylor Spatial Frame (TSF) at Nottingham Hospitals. The TSF is an external fixator system used to treat a range of fractures and limb deformities. Schanz pins, composed of stainless steel and coated with hydroxyapatite to enhance osseointegration, will be retrieved post-treatment following successful healing or adverse events such as infection, inflammation, or loosening. Our primary analysis employs ToF-SIMS and hybrid Orbitrap™ SIMS (OrbiSIMS), enabling high-resolution molecular mass spectrometry, 3D imaging, and depth profiling. We will characterise lipid and protein deposition profiles on retrieved pin surfaces, identifying molecular species associated with immune-evasive or pro-inflammatory responses. Specifically, we aim to quantify key phospholipids and fatty acids and correlate their presence with clinical outcomes. By linking molecular signatures to patient data, FIBRIS will elucidate how lipid and protein adsorption modulates immune responses at the biomaterial interface and inform future implant design strategies that minimise the FBR.

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Real-Time Vacuum-Compatible Paternò–Büchi Reaction Coupled with ToF-SIMS Imaging for Single-Cell Lipid C=C Isomer Analysis

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Real-time in situ characterization of lipid carbon-carbon double bond (C=C) positional isomers at the single-cell level is of great significance for revealing cellular metabolic heterogeneity and understanding the pathological mechanisms of major diseases such as tumors[1]. To address the limitations of conventional offline Paternò–Büchi (PB) derivatization—including complex procedures, contamination risks, and loss of spatial resolution—this study developed a real-time, vacuum-compatible online PB photochemical derivatization mass spectrometry imaging platform integrated with Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS)[1][2].

As illustrated in Figure 1, a cyclic detection system integrating vapor-phase deposition, in situ reaction, and mass spectrometry imaging within a vacuum environment was designed. Using controllable vapor-phase deposition to deliver reagents onto sample surfaces and in situ ultraviolet excitation, real-time monitoring of lipid isomer derivatization was achieved. Standard compound validation confirmed efficient and dynamic photochemical reactions at the solid interface. The reaction process between oleic acid (OA) and 2-benzoylpyridine (2-BP) showed clear formation and accumulation of diagnostic adduct ions. Benefiting from the sputtering capability of ToF-SIMS, the method enables high-resolution 3D spatial imaging. Meanwhile, structural identification of lipid isomers can be achieved at the single-cell level while preserving native morphology.

This work provides a powerful tool for single-cell spatial metabolomics, with potential applications in metabolic reprogramming, biomarker discovery, and intercellular communication studies.

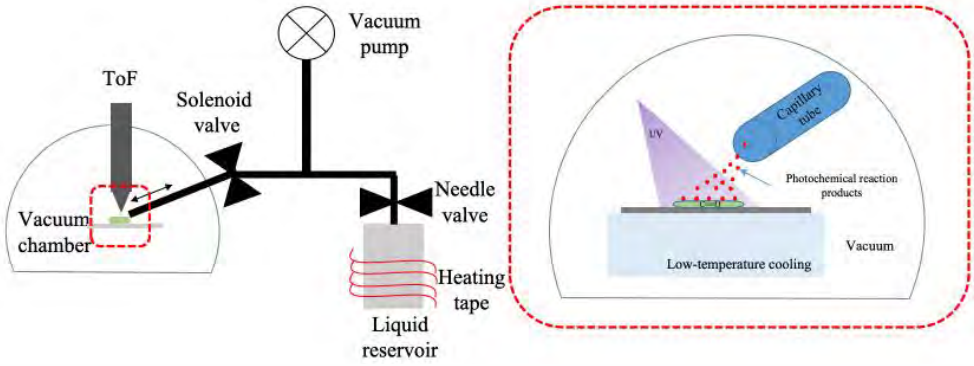


Figure 1. Schematic illustration of a vacuum-compatible system integrating vapor-phase deposition, in situ reaction, and ToF-SIMS imaging.

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Changes in Carbon Allocation during Tension Wood Formation

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Hardwood species, such as poplar, are known to form a specialized wood, termed tension wood, in response to stem inclination. Tension wood forms on the upper side of inclined stems, where xylem formation is enhanced and cellulose-rich wood is produced. The substantial accumulation of wood in this region suggests both increased cambial cell division and preferential allocation photosynthates. Understanding the mechanism behind tension wood formation provides critical insights into the regulation of biomass production in trees. In this study, we aimed to clarify asymmetric wood formation induced by stem inclination, focusing on changes in cambial activity and the allocation of photosynthates. We performed ^{13}C labeling using stable isotope-labeled carbon dioxide ($^{13}CO_2$) and analyzed the distribution of ^{13}C using Secondary Ion Mass Spectrometry (SIMS).

Poplar (*Populus alba* × *P. grandidentata*) shoots grown in a greenhouse were used. Stems were inclined at approximately 45°, and $^{13}CO_2$ was supplied 1 day to 2 weeks after the onset of inclination. Stems were then harvested, and small blocks of xylem including the cambial region were excised separately from the upper and lower sides. Samples were fixed with 4% paraformaldehyde and 2% glutaraldehyde, post-fixed with 1% osmium tetroxide, dehydrated through an ethanol series, and embedded in Spurr's resin. Sections were prepared, double-stained with 2% uranyl acetate and Reynolds' lead citrate and coated with platinum-palladium for conductivity. Observations were conducted using SEM, and ^{13}C distribution was analyzed using SIMS (NanoSIMS 50L, Cameca).

Changes in wood formation began to be observed around 2 days after the onset of inclination, and the differences between the upper and lower sides had become evident by 4 days. On the upper side, active cell division was observed, and the number of cells in the differentiating zone had already increased. As most of the newly formed cells were xylem fibers, the formation of vessel-poor wood, characteristic of tension wood, had already begun. ^{13}C labeling revealed that the preferential accumulation of photosynthates on the upper side, whereas little signal was detected on the lower side. These results indicate that asymmetric cambial activity and preferential allocation of photosynthates to the upper side are initiated shortly after stem inclination. We will also report the transport pathways of photosynthates revealed by ^{13}C distribution analysis, along with analyses of cell wall formation in tension wood.

Large-area Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) Imaging of the Human Growth Plate from Polydactyly Specimen

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The spatial organization of organic and inorganic components at the cartilage–bone interface in the human growth plate remains poorly understood. In this study, time-of-flight secondary ion mass spectrometry (ToF-SIMS) was applied for the first time to human growth plate samples to investigate these interfaces.[1] Three polydactyly specimens were analyzed to map spatial variations in hydroxyapatite and collagen-related components. Regions of interest were statistically evaluated using Dunn's multiple comparisons test and Spearman correlation analysis.

The calcified cartilage interface represents a critical transition zone, characterized by a sharp decline in organic matrix components (e.g., CH_4N^+) and a concurrent increase in mineral fragments ($CaPO_2^+$, Ca^+), particularly evident in large-area imaging. A pronounced peak in the Ca^+/CH_4N^+ ratio ($p < 0.0001$) highlights a rapid shift from organic-rich to mineral-rich composition. Correlations between organic (CNO^-) and mineral (PO_2^-) markers suggest early-stage mineralization, while the presence of phosphate and mineralized bone fragments confirms advanced mineralization in trabecular and cortical bone.

These findings are consistent with existing literature and support a structured, progressive mineralization pattern characteristic of endochondral ossification.[2-4] This study demonstrates the first application of ToF-SIMS to human growth plate samples from polydactyly cases, highlighting its capability for large-scale imaging of growth plate interfaces and its potential relevance for orthopedic research.

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Key words: TOF-SIMS, growth plate mineralization, endochondral ossification, organic matrix components, hydroxyapatite-fragment, collagen-fragment

Unsupervised Multi-Channel Clustering for Automated NanoSIMS Phase Mapping: A Scalable Python Workflow

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NanoSIMS provides high spatial resolution imaging of up to seven ionic species (channels) simultaneously. For all application areas, datasets are growing with increases in the number of samples to be analysed, increased numbers of species of interest, 3D data sets and more complex correlations of signals. Manual region of interest (ROI) generation therefore becomes slow and impractical and is liable to be biased by the user or complex correlations may be missed.

Hu et al. recently showed that K-means followed by Hierarchical Agglomerative Clustering (HAC) automates phase identification in soil samples analysed by NanoSIMS [1]. Here we extend this approach to engineering alloys with three advances: (i) six simultaneously acquired channels, doubling the original channel count; (ii) batch co-analysis of multiple independent measurements in one workflow run; and (iii) re-implementation in a new Python platform, replacing the R-based toolbox.

In this example an additively manufactured Al-Li alloy (AA2395) with extremely complex and diverse precipitate phases was analysed by NanoSIMS. The ionic species detected were $^{7}Li^{+}$, $^{24}Mg^{+}$, $^{27}Al^{+}$, $^{56}Fe^{+}$, $^{63}Cu^{+}$, $^{107}Ag^{+}$ across 4 different areas (craters). K-means (70 clusters, 20 initializations) over-segments all signals then HAC merges them into chemically distinct phase groups without prior compositional or phase information. The workflow identified 9 phases: the δ’ (Al_3Li) precipitate enriched in Li and Mg (HAC 1), Al-Cu particles (HAC 4), an Ag-rich phase (HAC 6), and the Al matrix (HAC 2), among others—all without user-defined constraints. Cross-measurement comparison (Figure 1) revealed pronounced heterogeneity: Craters 1 and 4 were δ’-dominated; Crater 2 showed significant Al-Cu contributions. The workflow was 20 times faster than manually identifying and drawing ROIs (3 min vs. ∼1 h for five craters) with rigorous phase quantification and the workflow identified phases that were missed during manual identification especially when the phases are defined by variations in more than 2 ionic species. The approach presented here can be extended to other multi-phase systems analysed by NanoSIMS.

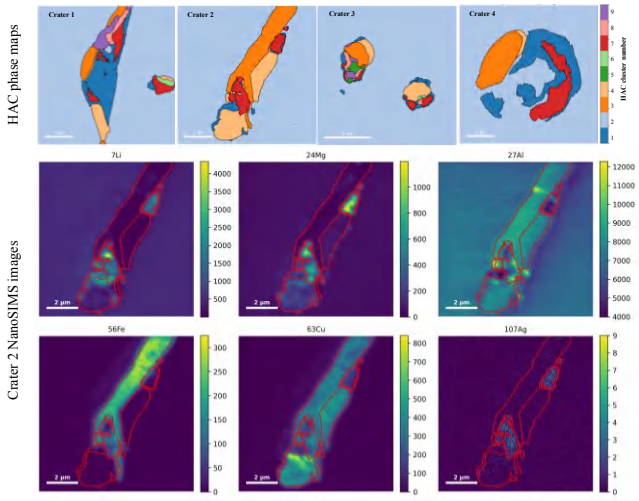


Figure 1. Top row: HAC-derived phase maps from four independent NanoSIMS measurements of the Al–Li alloy AA2395. Each color denotes a distinct compositional phase identified using the automated K-means/HAC workflow. Bottom two rows: Representative NanoSIMS total ion images from Crater 2 (selected isotopes shown), with red contours indicating HAC-derived phase boundaries corresponding to the phase map in the top row.

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Key words: NanoSIMS, K-means, HAC, Automated phase identification, Al-Li alloy

Combining unsupervised and supervised learning methods to analyse SIMS datasets of complex samples containing multiple organic molecules

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Data analysis techniques such as multivariate analysis, machine learning and deep learning [1-4] strongly support the interpretation of complex secondary ion mass spectrometry (SIMS) data. Unsupervised learning methods are useful for extracting important features or components, including unknown ones, from SIMS datasets of complex samples. Supervised learning methods are effective for searching for variables or samples related to a target factor. When samples including unknown factors are analysed, unsupervised learning methods may be first applied to the datasets of the samples. Once important factors have been identified, supervised learning methods can be applied to find variables related to these factors. Artificial neural networks (ANNs) are useful for approximating functions that express the physical or chemical laws behind sample data. As SIMS data often include nonlinear factors, such as matrix effects, ANN-based methods are effective for such datasets. These data analysis procedures were applied to datasets collected in two Versailles Project on Advanced Materials and Standards (VAMAS) projects: TW2 A26 [3] and A31 [4]. Peptide samples and organic electroluminescent (OEL) mixture samples were analysed in these projects. In addition to ANN-based methods, the supervised learning methods Random Forest [4] and the least absolute shrinkage and selection operator (LASSO) [5] were used. These supervised learning methods, including the ANN-based methods, can also provide information on the analysis processes, which is useful for understanding the relationships between the various factors involved. Even when the main molecules in a sample are known, suitable mass peaks for imaging or depth profiling are not always obvious. These supervised learning methods indicated fragment ions related to a molecule or a particular chemical structure that are useful for imaging or depth profiling. Furthermore, information entropy [6] and the Hopfield neural network [7] were applied to SIMS datasets in order to obtain a sample outline and evaluate the sample conditions.

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https://doi.org/10.1007/s44211-026-00916-y

Key words: machine learning, ANN, Peptide, OEL

ChASE: A Retrieval-Augmented AI Assistant for SIMS Method Development, Analysis Conditions, and Job Scheduling

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Secondary Ion Mass Spectrometry (SIMS) remains one of the most sensitive, but also one of the most analyst-dependent, techniques in materials characterization. Choosing a primary ion, energy, mass resolution, and raster; anticipating molecular interferences; accounting for tool history and potential carry-over contaminants; and translating a customer's need into a viable recipe all rely heavily on tacit knowledge that lives with individual scientists. We present ChASE (Chat-bot Augmented for SIMS Expertise), a chatbot-style AI assistant built specifically for easier training, faster recipe development, and more efficient scheduling in SIMS laboratories. ChASE couples retrieval-augmented generation (RAG) over a curated corpus of literature, internal standard operating procedures, and instrument documentation with large-language-model reasoning, and live integration with laboratory information management system (LIMS) information including a historical database of setup recipes.

The presentation will outline the underlying architecture and provide use cases demonstrated with real laboratory queries. Two classes of workflow are highlighted. The first is analyst-facing setup guidance: given a sample description, ChASE proposes primary beam conditions, sample high voltage, potential mass interferences, elements to monitor for the requested application, and likely contaminants based on the recent history of the chosen instrument, taking into account the requesting client's request and prior analyses. The second builds on the first: given the current job queue, the assistant drafts a schedule with time estimates informed by instrument status, ranked similar past setups and explicit prompt rules for prep, tuning, sputter time, repeats, and buffer to attempt to optimize use of available instruments. In the latter case, the instrument setup capabilities of ChASE are used to consider tradeoffs between finding common setups among analyses and providing the best quality data.

We discuss the intended role of the tool across the expertise gradient — from training newer analysts via a grounded, cited starting point, to providing optimization assistance and surfacing less-obvious options to experienced analysts — and share concrete examples where the assistant was clearly useful, where its suggestions were partially correct, and where it missed the mark entirely. These failure modes motivate a human-in-the-loop framing and an ongoing evaluation program as the corpus and historical setup coverage expand. To our knowledge this is the first domain-specific SIMS assistant of its kind, and we invite discussion on evaluation, safety, and appropriate reliance in SIMS laboratories.

Interface evaluation of organic electroluminescent (OEL) mixed layers by analysing depth profiles using supervised machine learning

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Matrix effects [1-4] cause changes in mass peak intensities that are independent of analyte concentrations, thereby reducing the quantitative accuracy of secondary ion mass spectrometry (SIMS). For solid samples, internal standard methods are difficult to apply, and reliable correction of matrix effects remains a major challenge. In SIMS, quantification methods based on relative sensitivity factors have been proposed [2,3]. However, these methods require peaks that strongly depend on concentration, and are not always applicable to complex or unknown samples. In this study, we applied an artificial neural network (ANN)-based supervised learning system developed for quantitative analysis for SIMS spectra affected by matrix effects [4,5] to the depth profiles of a multilayer sample. This sample contained mixtures of two organic electroluminescent materials, $Ir(ppy)_3$ and Alq_3, which was prepared under the Versailles Project on Advanced Materials and Standards (VAMAS), project TWA2 A31 [4]. In the previous study, positive ion datasets were used for the quantitative analysis by the ANN system. To improve prediction accuracy for the inside of a layer, positive and negative secondary ion combined datasets were used. While the mixtures were predicted correctly, predicting interfaces proved challenging in the previous study [4] due to the limited range of mixing ratios for standard samples (increments of 0.25), which made it difficult to accurately predict concentration changes, especially at the interfaces. To address this problem, X-ray photoelectron spectroscopy (XPS) depth profiles of the same samples were used to teach the ANN system to predict SIMS depth profiles of the interfaces.

Acknowledgements:

We thank the participants of the VAMAS TWA2 A31 project.

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Application of Generative AI-based Data Augmentation for Organic Contaminant Identification on TOF-SIMS in Advanced Semiconductor Manufacturing

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Organic contaminants adsorbed on wafer surfaces can adversely affect device performance, chip yield, and reliability, particularly in scaled leading-edge nodes and advanced packaging with heterostructures. The development of effective techniques for the detection and source identification of these pollutants is therefore crucial for high-quality fabrication. While artificial intelligence (AI) has emerged as an effective tool for processing and analyzing such complex micro-contamination data, practical applications often face the challenge of data scarcity for critical contaminants. This lack of sufficient training instances for key substances leads to highly imbalanced data distributions, which severely limits the model's ability to extract features and accurately identify these critical pollutants.

To address this training data deficiency, our team proposes an auxiliary solution based on generative AI (e.g., Generative Adversarial Networks, GANs). This tool is capable of generating highly realistic and diverse feature data for minority classes of critical pollutants, effectively filling the data gaps in the training set. In our experimental design, the GAN-generated data is integrated and evaluated across five pre-trained multi-label classification models, each designed to detect two specific target contaminants. By assessing the performance after incorporating the generated data, this study aims to validate how generative AI can effectively enhance the classifier's sensitivity and overall accuracy for scarce contaminants. This approach provides a more robust AI detection framework for precise contamination control in advanced manufacturing processes.

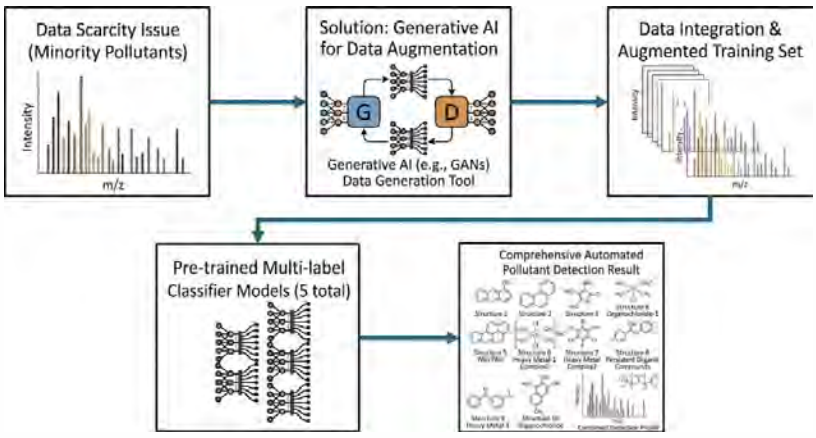


Figure 1. An integrated framework for minority pollutant detection via GAN-driven mass spectrometry data augmentation and multi-label classification.

Algorithmic Developments for ToF-SIMS Bioanalysis: 3D Tissue Imaging, Multi-Mode Fusion, High-Throughput Single-Cell Profiling and SVR-Based Batch Effect Correction

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Minzu University of China

ToF-SIMS enables label-free, *in situ* molecular imaging with high spatial resolution and chemical specificity, making it highly promising for biological and biomedical applications. However, its practical performance is still limited by several key challenges, including insufficient three-dimensional reconstruction for tissue samples, inherent trade-offs between mass resolution and spatial resolution in single-cell imaging, low analytical throughput for large cell populations, and technical batch effects that compromise data reproducibility.

To address these bottlenecks systematically, we present a suite of integrated algorithmic developments for ToF-SIMS bioanalysis. First, we developed a dedicated 3D mass spectrometry imaging algorithm for tissue sections, which enables high-resolution volumetric reconstruction of brain tissue and reveals the 3D spatial distribution of biomolecules within the native tissue microenvironment. Second, we proposed a multi-mode data fusion algorithm that combines ToF-SIMS datasets acquired in high-mass-resolution and high-spatial-resolution modes. This approach effectively breaks the performance trade-off between the two modes, allowing simultaneous high-quality molecular identification and fine structural visualization at the single-cell level. Third, we established a high-throughput single-cell segmentation and profiling algorithm with nucleus-level resolution, which supports in situ molecular imaging and phenotypic classification of tens of thousands of cells in a single experiment, significantly improving throughput and statistical reliability for heterogeneous sample analysis. Additionally, we introduced a metabolomics-inspired support vector regression (SVR) correction method for ToF-SIMS single-cell data, which effectively removes batch effects and technical variations, enhancing data consistency and quantitative accuracy.

Collectively, these algorithmic advances extend ToF-SIMS capabilities from 2D surface imaging to 3D tissue reconstruction, from single-mode constrained measurements to dual high-resolution imaging, and from low-throughput analysis to high-throughput in situ cell typing, with robust batch-effect correction ensuring reliable quantitative results. This integrated framework provides a powerful methodological platform for ToF-SIMS applications in neuroscience, single-cell biology, and biomedical research.

Key words: ToF-SIMS; 3D Imaging; Data Correction; High Throughput; Single Cell Imaging.

Multimodal and AI-driven TOF-SIMS: Advancing battery interface research from static snapshots to dynamic visualization

Jie Liu[a, b], Ning Li[a *], Yuefeng Su[a *], Handong Liang[b *], ZhanPing Li[d *]

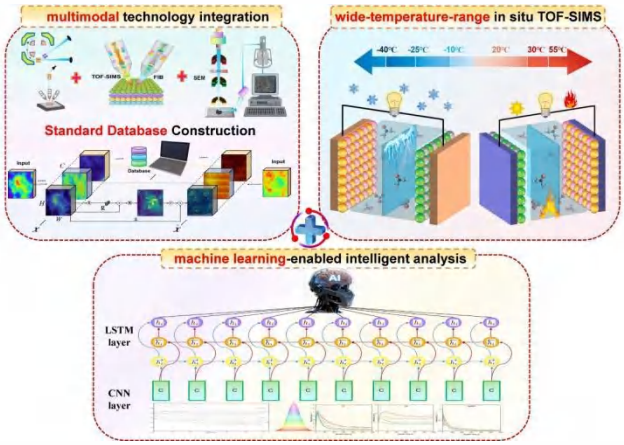
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Electrode–electrolyte interfaces are chemically heterogeneous and continuously evolving regions that govern ion transport, reaction kinetics, and battery degradation. Time-of-flight secondary ion mass spectrometry (TOF-SIMS) has emerged as a powerful technique for probing these interfaces. However, most TOF-SIMS analyses of battery materials are still performed ex situ under high-vacuum conditions. Consequently, the obtained chemical images usually represent discrete static snapshots at selected electrochemical states, rather than a continuous description of interfacial evolution. Additional challenges, including matrix effects, ion-beam-induced fragmentation, sputtering-related redistribution, and sample-transfer artifacts, further complicate the mechanistic interpretation of complex interphases.We present a multimodal and AI-driven TOF-SIMS framework for reconstructing battery interface evolution from discrete chemical information. TOF-SIMS datasets acquired at different cycling stages are treated as temporally correlated chemical fingerprints rather than isolated observations. Correlative characterization using X-ray photoelectron spectroscopy, focused ion beam-based sectioning and cryogenic transfer provides complementary chemical-state, structural, morphological and spatial information, improving the reliability of individual snapshots. Meanwhile, machine learning enables high-dimensional spectral interpretation, feature extraction, image clustering, and cross-modal data alignment. By incorporating physical constraints such as reaction kinetics, mass transport, and phase evolution, AI-assisted TOF-SIMS may bridge discrete observations with continuous interfacial dynamics, advancing TOF-SIMS from descriptive surface analysis toward an intelligent and predictive platform for battery interface science.

Keywords: TOF-SIMS; battery interfaces; solid electrolyte interphase; multimodal characterization; artificial intelligence; dynamic visualization;



LIMAS–New horizon of noble gas cosmochemistry

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Noble gases found in natural solids are used as tracers to study natural phenomena. However, the process by which they are incorporated into solids is not well understood. In this context, chemical thermodynamics is not very useful because the amount extracted from solids usually exceeds the amount that can be dissolved. If noble gases were trapped by adsorption, they would be found on the surface of or at the interface between solids. If noble gases were implanted into solids, they would be found just beneath the surface. In either case, microanalysis of noble gases in solids is essential to clarifying their incorporation mechanism. Recently, a novel in situ noble gas analysis technique using the Laser Ionization Mass Nanoscope (LIMAS) was developed [1]. LIMAS can conduct isotope measurements with lateral and depth resolutions of 10 nm and 5 nm, respectively, and down to ~1 atomic ppm (~10^{17} cm^{-3}) for ^{4}He with 1 μm resolution.

LIMAS measurements reveal the following novel astrophysical evidence: Presolar mainstream SiC grains form during the last million years of AGB stars and then migrate outward immediately. During this migration, the grains are irradiated by stellar winds from the central stars of planetary nebulae, at distances ranging from 0.3 to 30 light-years from their formation [2]. Solar wind components in meteorites are found in just below the solid surface, at depths of less than 100 nm, and the irradiated grains form a network structure generated by granular convection in the early solar system [3, 4, 5]. Solar wind components are significantly fractionated isotopically during their implantation, and solar energetic particles have not been observed in natural samples [6]. A large solar event, approximately 40 times larger than the largest solar particle ejection events observed since the space-based measurement of solar activity began, has been identified [7].

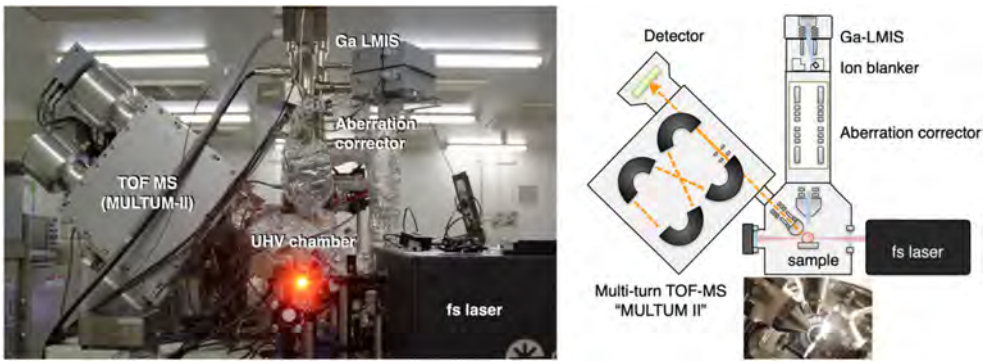


Figure 1. Photograph and schematic image of LIMAS. Configuration of primary and secondary columns and sample holder is inserted.

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Application of Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) in the Analysis of Organic Matter in Extraterrestrial Samples

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The analysis of organic matter in extraterrestrial samples is pivotal for understanding the evolution of prebiotic molecules and the origins of life in the solar system. However, characterizing these samples is hindered by their scarcity (milligram-level), low organic abundance (ppm-level), and complex matrices. Traditional techniques often fail to provide integrated multi-dimensional insights due to limited spatial resolution or the alteration of pristine states via solvent extraction. Consequently, there is an urgent need for highly sensitive, high-resolution, and non-destructive multimodal analytical strategies.

This study establishes a cross-scale multimodal imaging framework integrating vibrational spectroscopy with mass spectrometry imaging. This approach systematically overcomes critical bottlenecks, including contamination-free sample preparation, precise data registration, and matrix effect correction. Within this framework, Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) plays a pivotal role. Leveraging its ultra-high spatial resolution (<50 nm) and high sensitivity (ppb-ppm level), ToF-SIMS enables the precise sub-micrometer localization of trace organics. Furthermore, its surface sensitivity and ultra-high vacuum environment ensure the acquisition of pristine molecular information free from exogenous contamination. Uniquely, the integration of parallel imaging tandem mass spectrometry (MS/MS) allows for the simultaneous structural elucidation and visualization of complex organic molecules in a single analysis.

Applied to the Murchison meteorite, this workflow achieved a comprehensive resolution of mineral phases, functional groups, molecular compositions, and isotopic characteristics within 100-μm-scale micro-regions. Notably, this study marks the first use of the parallel imaging MS/MS function of ToF-SIMS for the structural and imaging analysis of organic components in meteorites, constructing a high-spatial-resolution organic-inorganic multi-dimensional correlation network[1]. These findings provide a robust methodological framework for the in situ, near-lossless, and multi-dimensional analysis of extraterrestrial samples.

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From Organic Matter to H_2: TOF-SIMS/XPS Insights into Thermally Driven Hydrogen Generation in Mudrocks

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Geologic hydrogen is attracting increasing interest as a potential low-carbon energy resource, but the role of sedimentary organic matter in hydrogen generation remains insufficiently understood. In this study, we investigate molecular hydrogen release from organic-rich carbonate mudrocks during thermal treatment, with emphasis on the molecular and surface transformations that control gas formation.

An integrated analytical workflow combining GC, TOF-SIMS, XPS, and FTIR spectroscopy was established. Gas analysis revealed substantial H_2 production together with light hydrocarbons and carbon oxides, consistent with coupled dehydrogenation, cracking, and decarboxylation reactions. TOF-SIMS provided surface-sensitive molecular evidence for progressive alteration of the organic matter, including depletion of aliphatic and oxygen-bearing fragments and enrichment of aromatic carbon-related signals. These observations were supported by XPS, which showed increased carbon enrichment and aromatic character, and by FTIR, which confirmed the loss of characteristic aliphatic and carbonyl functional groups.

The combined results show that hydrogen generation from organic-rich carbonate mudrocks is governed by thermal dehydrogenation, structural reorganization of organic matter, and mineral–organic interactions that may promote catalytic reaction pathways during pyrolysis. By linking gas evolution with TOF-SIMS/XPS-based molecular surface characterization, this study demonstrates the value of TOF-SIMS/XPS for resolving reaction mechanisms in complex geological materials. The findings provide experimental evidence that organic-rich sedimentary rocks can contribute to natural or stimulated hydrogen systems, broadening current perspectives on geologic hydrogen as part of future clean energy strategies.

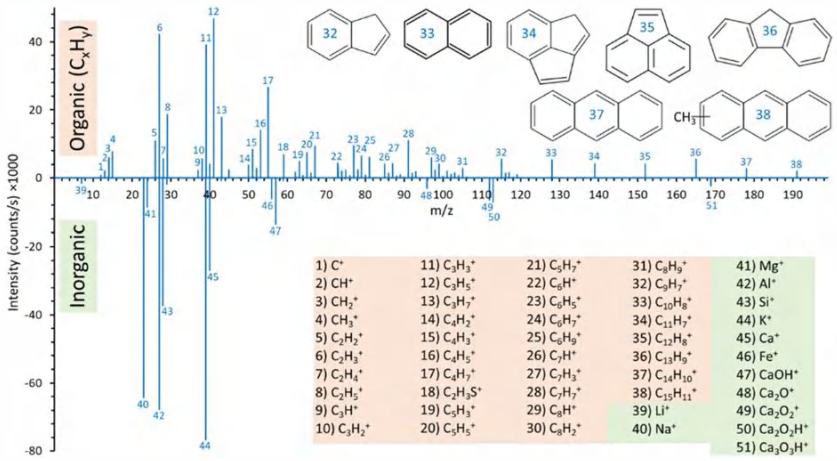


Figure 1. *The TOF-SIMS mass spectrum at 450 °C in positive ion mode minus the mass spectrum at 25 °C. All the ion intensities were normalized against the summed total ion intensity prior to being subtracted in order to remove possible instrument effects.*

MeV SIMS in a Multianalytical Protocol for Studying Colorant Mixtures and Lightfastness in Modern Writing and Acrylic Inks

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Analytical protocols used to investigate modern inks in heritage science are often adapted from forensic science but must address different constraints. While forensic analysis focuses on ink discrimination and authenticity [1], heritage science seeks maximum chemical information on ink stability from extremely limited samples while preserving object integrity. Modern inks are particularly challenging as they contain complex mixtures of synthetic organic colorants with binders and additives [2,3], often inaccessible by a single technique. Here, a minimally invasive multianalytical protocol combining secondary ion mass spectrometry with MeV primary ions (MeV SIMS)—an emerging technique in the field [4,5]—with μ-Raman spectroscopy and microfading testing (MFT) was applied for direct ink-on-paper analysis without chemical treatment, separation, or sample consumption.

The first study focuses on writing inks from ballpoint and fiber pens in literary works (1960s–2012) kept at the Austrian National Library. MeV SIMS enabled detection of cationic dyes and aryl guanidines as markers of anionic dyes, providing information complementary to μ-Raman. The technique proved particularly valuable for identifying synthetic dyes with similar molecular structures and aiding the interpretation of Raman results. MFT revealed moderate fading, with inks containing only anionic dyes exhibiting lower lightfastness. These results suggest that cationic–anionic dye mixtures may enhance light stability through dye–salt formation.

The second study presents the first systematic analysis of acrylic inks, focusing on synthetic organic pigments (SOPs) in inks originally used by the Austrian caricaturist Erich Sokol (1933–2003). Ink-on-paper mock-ups were aged by MFT, while selected sets were displayed for one year in a museum exhibition under different lighting conditions. MeV SIMS enabled identification of pigment mixtures and formulation differences that were unresolved by μ-Raman alone. Aging revealed chemical changes in several SOPs, particularly in mixtures where one pigment degraded faster, and showed that lighting conditions influence degradation. The protocol was applied to a minute sample from a Sokol caricature, demonstrating its suitability for minimally invasive SOP identification.

Together, these studies show that integrating MeV SIMS within a multianalytical protocol enables comprehensive molecular characterization of complex ink systems and their light stability while requiring minimal sampling from valuable heritage objects.

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Cryogenic SIMS for Preserving Intrinsic Elemental Distributions

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Materials exist under a wide range of environments, including planetary interiors, biological systems, and outer space; however, SIMS analyses are typically conducted under ultra-high vacuum at ambient temperature in the presence of high electric fields. In addition, sample preparation procedures are generally performed under ambient conditions. As a result, wet samples containing liquids under ambient conditions are difficult to analyze, and preserving elemental and isotopic distributions formed under extreme conditions where processes such as partitioning, phase transitions, or chemical reactions occur is even more challenging.

To enable such analyses, we established a fully cryogenic SIMS workflow (Cryo-SIMS), in which all processes, including sample preparation, transfer, and analysis, are performed under cryogenic conditions using liquid nitrogen to suppress atomic and molecular mobility. This approach effectively prevents elemental redistribution and enables preservation of original elemental and isotopic distributions. As a demonstration of this method, we quantified hydrogen in metal systems that incorporate hydrogen only under extreme conditions and rapidly lose it upon warming above −70 °C [1], clearly showing that cryogenic conditions must be maintained below this temperature throughout the entire workflow to preserve the original elemental distributions.

The developed Cryo-SIMS technique enables high-sensitivity analysis of volatile elements and isotopes while preserving their original distributions, with submicron lateral spatial resolution and nanometer-scale depth resolution. This approach provides a robust analytical platform for functional, biological, and terrestrial/extraterrestrial materials.

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Multimodal FIB-SIMS Workflow for Interfacial and Lithium Transport Characterisation in PEO–LLZO Hybrid Solid Electrolytes

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The development of advanced polymeric materials has gained increasing interest across multiple disciplines, particularly within the field of battery technology. Nanoscale chemical heterogeneity and the dynamic behaviour of lithium transport, including within polymer electrolytes and hybrid solid electrolytes (HSEs), remain poorly understood. Mainly due to the fact that conventional characterization methods lack the spatial resolution and sensitivity required to resolve lithium diffusion pathways at the relevant length scales.

To address these analytical challenges, the Luxembourg Institute of Science and Technology (LIST) has developed multimodal imaging platforms that integrate magnetic sector SIMS with high resolution focused ion beam (FIB) columns, enabling advanced in situ correlative microscopy. More specifically, the system employed in this work is a helium ion microscope (HIM) that uses a gas field ion source (GFIS) column, which provides a highly focused ion probe (e.g. He^+ or Ne^+) with sub-nanometre beam diameters. This is particularly advantageous for SIMS applications, as it enables exceptional lateral resolution while maintaining high surface sensitivity, thereby making it especially well-suited for nanoscale chemical imaging of complex materials systems. In secondary electron (SE) imaging mode, sub-nanometre spatial resolution can be achieved, enabling detailed morphological analysis. In SIMS mode, the system attains lateral resolutions down to 15 nm while preserving high sensitivity [1]. Such performance enables spatially resolved detection of isotopes and trace elements, including isotopic analysis, thereby opening new possibilities for nanoscale investigations of material interfaces, chemical heterogeneities among others [2].

In this study, we apply this platform through a novel experimental workflow for the characterisation of HSEs in PEO(LiTFSI)–LLZO symmetric cells at different stages of electrochemical cycling. First, Li^{nat}/HSE/Li^{nat} (Li^{nat} stands for natural abundance lithium electrodes) symmetric cells were employed to correlate solid electrolyte interphase (SEI) growth, overpotential, and chemical degradation with the chemical structure obtained from SIMS imaging analysis. Subsequently, the capability of SIMS to distinguish light isotopes was exploited using Li^{nat}/HSE/^{6}Li (^{6}Li stands for Lithium6-rich (95%) electrodes) symmetric cells, enabling the investigation of lithium trapping and providing new insights into ion transport across the different phases. Overall, this workflow offers an unprecedented combination of sensitivity, isotopic selectivity, and spatial resolution for studying complex interfacial processes and transport mechanisms in solid electrolytes, demonstrating the capabilities of this multimodal FIB-SIMS platform for advanced HSE characterisation, providing a powerful framework for understanding interfacial processes and offering researchers a decisive new tool to engineer the next generation of solid-state batteries.

This work was co-funded by the Luxembourg National Research Fund (FNR) through the grant INTER/DFG/22/16558792/MINABATT and the German Research Foundation (DFG) HE8586/MINABATT.

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Unveiling the Role of Hydrogen in the Dielectric of PEALD AlBN Ultra-Thin Films via TOF-SIMS Depth Profiling

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Aluminum boron nitride (AlBN) is an emerging high-k dielectric featuring superior thermal conductivity and suppressed remote optical phonon scattering. However, optimizing plasma-enhanced atomic layer deposited (PEALD) AlBN remains challenging. We found that as-deposited AlBN metal-insulator-semiconductor (MIS) structures on heavily doped Si substrates ($\rho < 0.005\ \Omega \cdot$ cm) consistently exhibit anomalous S-shaped capacitance-voltage (C-V) curves. Physically, such voltage-dependent distortions are typical macroscopic signatures of high-density border traps and slow charge-responsive states. To elucidate the chemical origin of these localized states, time-of-flight secondary ion mass spectrometry (TOF-SIMS) was utilized to track the relative depth distribution and thermal evolution of light-element impurities. Comparative TOF-SIMS depth profiling reveals that the reducing PEALD plasma introduces substantial hydrogen throughout the film bulk. Supported by XPS identification of N-H bonding states, we verify that this incorporated H acts as a structural terminator. It not only generates parasitic charge-trapping sites but also chemically hinders the cross-linking of the robust Al-B-N covalent network, thereby suppressing its intrinsic dielectric polarizability. Upon 650 ℃ rapid thermal annealing (RTA), TOF-SIMS captures the dynamic out-diffusion of hydrogen, evidenced by a pronounced relative decrease in the bulk H^- secondary ion intensity. This micro-chemical H-escape precisely coincides with the complete macroscopic elimination of the C-V distortion, recovering a highly stable, voltage-independent capacitance behavior alongside a significantly enhanced capacitance density.. Ultimately, TOF-SIMS relative profiling unequivocally correlates thermal H desorption with the covalent densification and trap passivation of PEALD AlBN, providing a fundamental pathway to restore its intrinsic dielectric reliability.

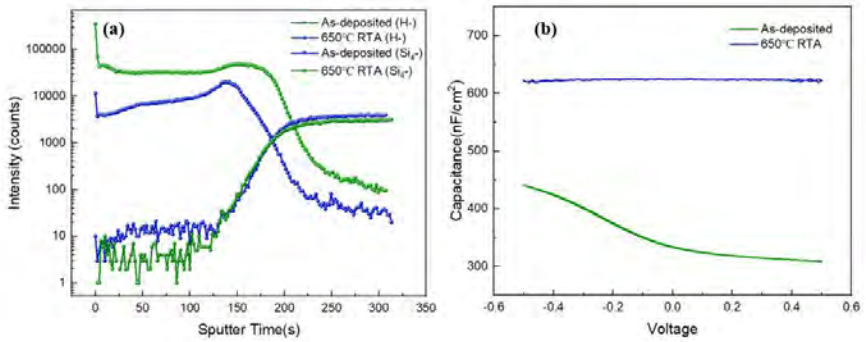


Figure 1. (a) Comparative TOF-SIMS depth profiles of AlBN films. Using Si4− as an interface marker, a pronounced relative decrease in bulk H− intensity is observed after 650 °C RTA. (b) Corresponding C−V curves demonstrating the transition from a trap-induced distortion to a flat, intrinsic dielectric plateau with enhanced capacitance.

High-Sensitivity, In Situ Analysis of Hydrogen Using Dynamic SIMS

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O. Dulac[1], T. Faye[1], Y. Wang[2], A. Jiao[2], J. Bai[2], A. Zou[2]

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Hydrogen is the most abundant element in the environment and can be incorporated into materials either intentionally, during epitaxy, ion implantation, and thermal treatments, or unintentionally through environmental exposure or process-induced contamination. Because hydrogen can strongly influence electrical, mechanical, and reliability-related properties, accurate characterization of its distribution at both the micron and nanometer scales remains a critical challenge in semiconductor and functional materials research.

Dynamic SIMS is a reference technique for hydrogen analysis thanks to its unrivaled sensitivity, wide dynamic range, and versatility for depth profiling and imaging. Implemented on magnetic-sector instruments, it provides the highest sensitivity for hydrogen and other light elements, enabling ppm-level (and below) detection limits while maintaining excellent depth resolution. CAMECA has developed several state-of-the-art magnetic-sector SIMS instruments optimized for different analytical needs.

In this work, we illustrate the capabilities of magnetic-sector dynamic SIMS for hydrogen analysis using two complementary CAMECA platforms. High-throughput depth profiling applications are demonstrated using the IMS 7f-Auto, highlighting reliable hydrogen quantification across a wide range of concentrations and depths relevant to semiconductor process control and advanced materials development. High spatial-resolution hydrogen mapping is addressed using the NanoSIMS-HR, whose combination of high lateral resolution, high mass resolving power, and multicollection enables nanoscale investigation of hydrogen distributions and local chemical environments in complex materials and device architectures.

Through selected application examples, this contribution demonstrates how dynamic SIMS continues to expand the analytical window for hydrogen characterization, enabling both routine process monitoring and advanced investigations of hydrogen-related phenomena in ion-implanted and nanostructured materials.

Characterization of composite materials dedicated to the extraction of lithium: a $^{6/7}$Li isotopic study by ToF-SIMS and neutron tomography

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Composites materials dedicated to the extraction of lithium from brines were synthesized. They consisted of lithium/aluminum layered double hydroxides (Li/Al-LDHs), a lithium adsorbent material exhibiting high extraction capacity and selectivity, [1,2,3] dispersed within a mesoporous geopolymer matrix. Geopolymer does not adsorb lithium but provides a porous network that facilitates brine transport toward Li/Al-LDHs particles, where adsorption occurs.
To investigate the lithium adsorption mechanisms, an innovative approach based on $^{6/7}$Li isotopic labeling was employed. The composites were exposed to ^{6}Li-enriched synthetic brines containing dissolved ^{6}LiCl. High-resolution ToF-SIMS imaging and neutron tomography were employed to study adsorption under various temperature and salinity conditions. The increase in the ^{6}Li isotopic ratio measured by ToF-SIMS within the Li/Al-LDHs phase over time confirmed effective lithium adsorption from the brine. Line-scan analyses revealed spatial heterogeneity in the adsorption, with a higher ^{6}Li enrichment near the outer regions of the composite than in the core. This heterogeneity was confirmed by the whole composite volume investigation in neutron tomography (Fig.1) where neutron attenuation, directly related to ^{6}Li presence, was significantly higher at the sample periphery than in the central region.
These observations indicated that the brine requires time to penetrate the entire mesoporous network and reach the Li/Al-LDHs particles located in the core of the composite. This highlights the importance of balancing adsorption kinetics and efficiency to optimize lithium extraction.

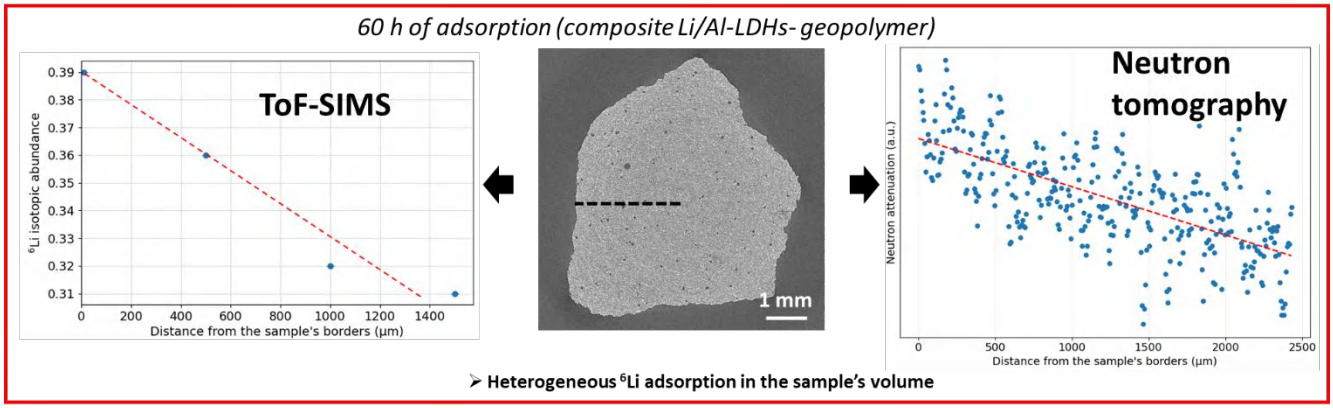


Fig. 1: Neutron tomography analysis of a composite after 60 h of adsorption

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Revealing Battery Interface Chemistry with High-Selectivity, Depth-Resolved ToF-SIMS Analysis

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Time-of-flight secondary ion mass spectrometry (ToF-SIMS) has established itself as one of the most powerful analytical tools in battery research, offering a unique combination of extreme surface sensitivity, outstanding chemical selectivity, and nanometer-scale depth-profiling capability. These attributes make it exceptionally well suited for elucidating the complex surface films, buried interfaces, and reaction gradients that govern the performance and stability of electrodes and electrolytes. Because ToF-SIMS instrumentation is rarely housed within battery research laboratories, most investigations rely on collaborations with specialized surface-analysis centers — a model that provides battery researchers access not only to state-of-the-art instrumentation but also to expert guidance in data interpretation, enabling mechanistic insights into interfacial phenomena that are otherwise inaccessible.

A widely held assumption in the field is that the discharge product of all-solid-state lithium-sulfur batteries consists solely of Li_2S. We demonstrate how ToF-SIMS enables direct identification of the previously overlooked intermediate Li_2S_2 as an additional discharge product. By evaluating the intensity ratio of $Li_3S_2^+$ to Li_3S^+, ToF-SIMS provides unambiguous chemical evidence for the coexistence of both species [1]. Recognition of Li_2S_2 has since motivated new strategies in which the Li_2S_2/Li_2S balance is deliberately manipulated to enhance electrochemical performance. Beyond discharge products, the surface chemistry of a cathode strongly influences its interaction with the electrolyte, typically giving rise to ultrathin interphase layers whose composition and structure directly impact electrochemical behavior. Depth-resolved characterization of these layers is therefore essential for understanding interfacial reactions in both liquid- and solid-state systems. We present two representative cases in which ToF-SIMS depth profiling revealed (i) the formation of an aluminum fluoride-rich passivation layer on a Li- and Mn-rich layered oxide cathode [2], and (ii) the development of a chemically distinct interfacial layer between electrode and solid-state electrolyte, permitting direct examination of soft-breakdown mechanisms [3].

Collectively, these examples illustrate the power of ToF-SIMS for advancing mechanistic understanding of electrochemical interfaces, and affirming its essential role in the guiding and optimization of next-generation battery materials.

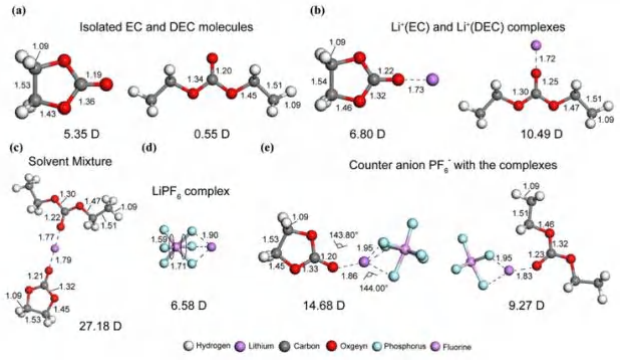
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Combining ToF-SIMS Depth Profiling and DFT Calculations to Elucidate Solid Electrolyte Interphase Formation in Lithium-Ion Batteries

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The solid electrolyte interphase (SEI) formed on graphite anodes plays a critical role in the performance and lifetime of lithium-ion batteries. However, its formation mechanism remains difficult to resolve because of its nanoscale heterogeneity and complex chemistry. In this work, time-of-flight secondary ion mass spectrometry (ToF-SIMS) depth profiling is combined with density functional theory (DFT) calculations to investigate SEI formation in $LiPF_6$-based electrolytes containing ethylene carbonate (EC) and diethyl carbonate (DEC). ToF-SIMS depth profiles, analyzed using principal component analysis, reveal a layered SEI structure consisting of an outer organic-rich porous region and an inner inorganic-rich compact layer. Organic fragments associated with carbonate decomposition products dominate the outer region, while lithium-containing species such as Li_2O^- and Li_2^- become more prominent near the electrode interface. To interpret these observations, DFT calculations were performed on Li^+ solvation complexes containing EC, DEC, and PF_6^-, as well as their adsorption on graphene as a model graphite surface. The results show that EC-rich Li^+ solvation structures are energetically favored and exhibit stronger adsorption and charge transfer than PF_6^--containing ion pairs. These findings indicate that Li^+-coordinated EC species are likely precursors for the initial reduction reactions leading to SEI formation. The combination of ToF-SIMS chemical depth profiling and DFT modeling provides a molecular-level description of SEI evolution and demonstrates how first-principles calculations can support the interpretation of complex SIMS data from electrochemical interfaces.



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Probing the Interfacial Growth and Layer-by-Layer Assembly of Surface-Supported MOFs via ToF-SIMS

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While metal–organic frameworks (MOFs) are celebrated for their tunable porosity and chemical versatility, their transition from bulk powders to integrated device components requires precise control over immobilization on solid substrates.

This study investigates the fabrication of surface-supported MOFs (sur-MOFs) using a layer-by-layer assembly approach, focusing on a copper-based system grown on SiO_2 substrates functionalized with a zirconium phosphate anchoring interlayer. We demonstrate that Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) provides a definitive molecular fingerprint of the assembly process, enabling the tracking of specific secondary ions—including metal clusters, organic linkers, and intact metal-organic coordination fragments—at the sub-nanoscale. The stepwise deposition was monitored after each growth cycle, allowing to correlate the attenuation of substrate-specific signals with the increase in MOF-related molecular fragments, thereby quantifying the film's thickness and growth. These results were correlated with X-ray photoelectron spectroscopy (XPS) and atomic force microscopy (AFM) to validate chemical states and morphological evolution.

This work underscores the power of SIMS-based characterization approaches for resolving the early-stage interfacial chemistry of complex hybrid nanostructures and guiding the precision fabrication of such materials for advanced device applications.

Acknowledgments
This work was partially supported by the project PRIDE (MASE Prog. n. RSH2A_000037 - CUP: F57G25000320006), the European Union's Horizon Europe research and innovation programme under the EIC Pathfinder Open project ERMES – Information Transfer Between Medical Doctors and Implanted Medical Devices via Artificial Molecular Communication (Grant Agreement No. 101185661) and the research project PIACERI 2024-2026 - Linea 1.

ToF-SIMS and XPS characterization on functional nanocoatings deposited on medical devices

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We report the results of an active collaboration between the University of Namur and Laval University on the development of novel plasma-deposited ultrathin coatings for medical devices, with a strong emphasis on characterization by time-of-flight secondary ion mass spectrometry (ToF-SIMS). Two case studies are presented: (i) compositionally graded coatings for dental implants and (ii) amorphous carbon coatings on PDMS-based medical devices.

Up to 20% of titanium alloy dental implants suffer from complications related to failed osseointegration or bacterial infection. There is therefore a critical need for bioactive coatings combining osteogenic and antibacterial properties. We have developed coatings deposited by plasma-enhanced chemical vapor deposition (PECVD) using a Ti-based organometallic precursor vapor mixed with argon and oxygen [1]. High oxygen flux yields titanium oxide coatings, while low oxygen flux produces carbon-rich TiO_xC_y films. Gradient coatings were achieved by progressively decreasing the oxygen flux, resulting in a mineral composition at the implant interface and a more organic composition toward the bone-facing surface, designed to promote osseointegration. An additional antibacterial layer of ZnO nanoparticles was deposited by magnetron sputtering. XPS depth profiling confirms a pronounced carbon gradient from the implant to the surface, rising from 10 to 30 at.%. ToF-SIMS depth profiling using 500 eV Cs^+ ions provides detailed insights into the coating's molecular structure. Characteristic ions of polymerized organometallic precursors (e.g. $TiC_2O_2H_2^-$) exhibit a pronounced but not linear gradient, indicating a competition between layer growth and plasma etching. ToF-SIMS also reveals evidence for hydrogen and carbon implantation into the titanium alloy.

In the second study [2], hydrogenated amorphous carbon (a-C:H) coatings were deposited by PECVD on PDMS substrates used in medical devices such as catheters and soft implants, with the goal of enabling controlled release of antibacterial agents. Coatings were deposited under four conditions, with or without substrate bias and with or without hydrogen addition. ToF-SIMS 3D analysis shows successful deposition of a-C:H layers but highlights significant PDMS diffusion through coating defects. The best coatings were obtained without substrate bias and without hydrogen addition, whereas biased deposition in the presence of hydrogen led to severe PDMS–carbon intermixing.

[1] S. Rubio, P. Chevallier, D. Mantovani, L. Houssiau, Coatings 16, 2026, 312.
[2] L. A. Yáñez-Hernández, et al., Applied Surface Science Advances 32, 2026, 100949.

Correlative SIMS techniques for semiconductor materials and applications

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The semiconductor landscape is rapidly evolving, driven by increasing demands for device performance, sustainability, and continued miniaturization. Beyond conventional silicon-based technologies, materials such as graphene and transition metal dichalcogenides (TMDs) are gaining increasing relevance for future device concepts. Their reduced dimensionality and sensitivity to interfaces, contamination, and processing conditions pose significant challenges for characterization. These systems require analytical approaches capable of providing high spatial resolution, excellent surface sensitivity, and unambiguous chemical identification.

Secondary Ion Mass Spectrometry (SIMS) is well suited to address these demands. Time-of-Flight (ToF) SIMS enables high-resolution chemical imaging and depth profiling, while high mass-resolving approaches such as Orbitrap^{TM}-SIMS provide enhanced mass accuracy and improved capability to resolve complex chemical signatures [1]. In addition, the integration of in-situ Scanning Probe Microscopy (SPM) offers complementary structural, electrical and topographical information, enabling for example a direct correlation between chemical and morphological features [2].

In this contribution, correlative SIMS approaches for the investigation of semiconductor-relevant material systems will be presented. Emphasis will be placed on the combination of conventional ToF-SIMS for high-resolution imaging and depth profiling, Orbitrap^{TM}-SIMS for advanced and unambiguous chemical identification, and in-situ SPM for nanoscale structural and electrical characterization.

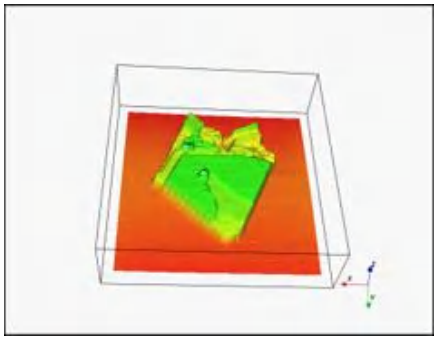


Figure 1. 3D correlation of the in-situ SPM topography information and the chemical mapping from ToF-SIMS acquired on a mechanically exfoliated MoS_2 flake.

[1] A. Franquet, V. Spampinato, S. Kayser, W. Vandervorst and P. van der Heide, Vacuum 202, 2022, 111182.
[2] V. Spampinato, M. Dialameh, A. Franquet, C. Fleischmann, T. Conard, P. van der Heide, and W. Vandervorst, Analytical Chemistry 92(16), 2020, 11413-11419.

Coupling Cryo-FIB-SEM with Orbitrap MS for Correlative Molecular and Electron Microscopy Imaging

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Secondary ion mass spectrometry (SIMS) and electron microscopy (EM) provide complementary insights into chemical composition and nanoscale structure. While integrated FIB-SEM-SIMS platforms have enabled elemental and limited molecular imaging, achieving high mass resolution molecular analysis within such systems remains a significant challenge. Here, we present ongoing development of a cryo-compatible interface coupling a focused ion beam–scanning electron microscope (FIB-SEM) to a high-resolution Orbitrap™ mass spectrometer (MS), to enable correlative molecular and electron microscopy imaging.

A custom secondary ion extraction and transfer system derived from a sector-based FIB-SEM-SIMS architecture [1] has been integrated into a cryo-FIB-SEM platform. This system directs secondary ions generated in the cryogenic FIB-SEM environment toward a dedicated transfer interface connected to a Thermo Scientific™ Orbitrap Exploris™ 480 mass spectrometer. The transfer interface incorporates collisional cooling to reduce the kinetic energy of the secondary ions prior to injection into the mass spectrometer. System performance has been evaluated through direct ion current measurements.

Recent results demonstrate successful end-to-end coupling of the FIB-SEM platform to the Orbitrap mass spectrometer. Using a CsI-coated grid as a model system, stable ion signals corresponding to CsI-derived species were observed during focused ion beam scanning, confirming continuous ion generation, transport, and detection within the integrated system. These measurements represent a key step toward fully functional molecular SIMS analysis with high mass resolving power in a cryogenic FIB-SEM environment.

Ongoing work focuses on characterizing ion energetics using retarding voltage analysis and optimizing ion transfer and cooling conditions. In parallel, proof-of-concept experiments are being developed to align Orbitrap MS acquisition with FIB scanning in order to reconstruct spatially resolved molecular images and correlate them with electron microscopy data.

This work establishes the feasibility of combining high-resolution Orbitrap-based molecular analysis with cryo-FIB-SEM and represents a significant step toward multimodal, correlative MS–EM imaging. The approach has the potential to enable detailed chemical and structural characterization of complex biological and materials systems at the nanoscale.

[1] De Castro, O; Audinot, J.-N.; Hoang, H. Q. et al. *Anal. Chem.* **2022** 94, 30, 10754–63.

Development of Operando MeV-SIMS Analytical Technique for Lithium-Ion Batteries

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Lithium-ion batteries (LIBs) have become widely used in various applications, particularly in portable devices such as laptops and smartphones. However, the internal reactions occurring within these rechargeable batteries are not yet fully understood. The solid–liquid interface represents the most critical boundary in electrochemical systems. For instance, a solid–electrolyte interphase (SEI) forms primarily at the interface between the LIB negative electrode (anode) and the electrolyte during charging. The SEI consists of reductive decomposition products of electrolyte molecules (including solvents, additives, and anions), resulting in a complex mixture of inorganic and organic substances. Because the SEI significantly influences LIB performance and safety, clarifying the reactions at the electrode–electrolyte interface, including SEI formation, is essential for further battery optimization.

This study establishes an operando MeV-SIMS analytical technique to investigate the SEI on LIB anodes. Traditional vacuum-based SIMS techniques are limited in assessing real-time solid–liquid interface reactions. To overcome this limitation, we developed a specialized sample holder featuring a pinhole through the cathode and separator, allowing high-energy (6 MeV Cu^{4+}) primary ion beams to probe the anode surface under atmospheric pressure. This approach enabled the successful tracking of SEI formation and evolution in real-time. Our results demonstrate that MeV-SIMS can distinguish between transient intermediate products and stable SEI components based on their distinct spectral intensity behaviors during electrochemical cycling. This innovative operando measurement platform provides a foundation for the molecular-level analysis of battery interfaces, thereby contributing to the development of next-generation, high-performance LIBs.

Acknowledgments

This research was supported by a 2024 research grant from the Suzuki Foundation (Project Title: Development of LIB electrolyte-electrode interface analysis technology using atmospheric pressure MeV-SIMS).

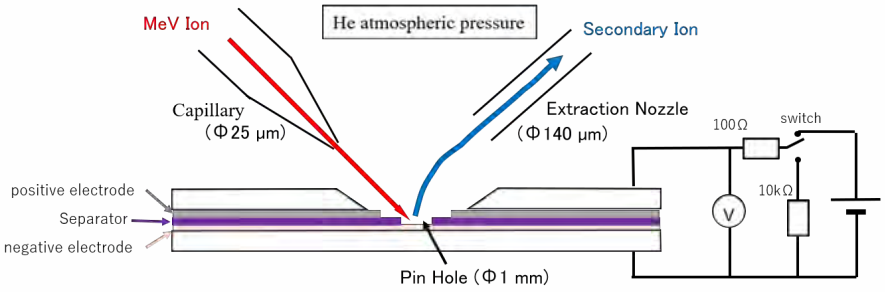


Fig.1 Schematic diagram of a holder specifically for operando MeV-SIMS measurement.

TOFSIMS and sMIM Multi-modal analysis on InGaP superlattices

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Time-of-flight secondary ion mass spectrometry (TOF-SIMS) provides high-resolution chemical depth profiling of semiconductor heterostructures, but its impact increases when compositional information is embedded in a broader correlative workflow. Here, we present a methodology that combines cluster-ion TOF-SIMS with cross-sectional vector based high resolution scanning microwave impedance microscopy (sMIM) [1], executed on an InGaP/GaAs superlattice with 30 nm / 5 nm period as a model system. Fig 1a shows cross-sectional sMIM conductance data on the InGaP:GaAs stack. Capacitance data (not shown) was dominated by geometry artifacts modulated by the local composition. TOF-SIMS was used to perform depth profiling using a $C60^+$ primary ion beam, chosen to mitigate ion-beam–induced mixing and damage relative to monoatomic sources while maintaining practical sputter rates for sub-micrometer stacks. Fig 1b shows normalized intensity profiles for InGaP- and GaAs-related secondary ions, together with oxygen-containing species. As the material was grown by Metal-Organic Vapor Phase Deposition, oxygen should not there be present, and it is related to residual gas inside the chamber as well as redeposited oxygen from adventitious water and native oxides. We could resolve the multilayer sequence and define a chemically referenced depth axis that serves as the backbone for subsequent correlative analysis. These profiles were directly compared with the conductance and capacitance profiles allowing for evaluation of TOF-SIMS-derived depth resolution. Our system is a IonOptika J105, the first TOFSIMs operational in Brazil, and these are the first results of the system. We thank the entire IonOptika team for technical support, FINEP, CNPq, CAPES and FAPEMIG for financial support.

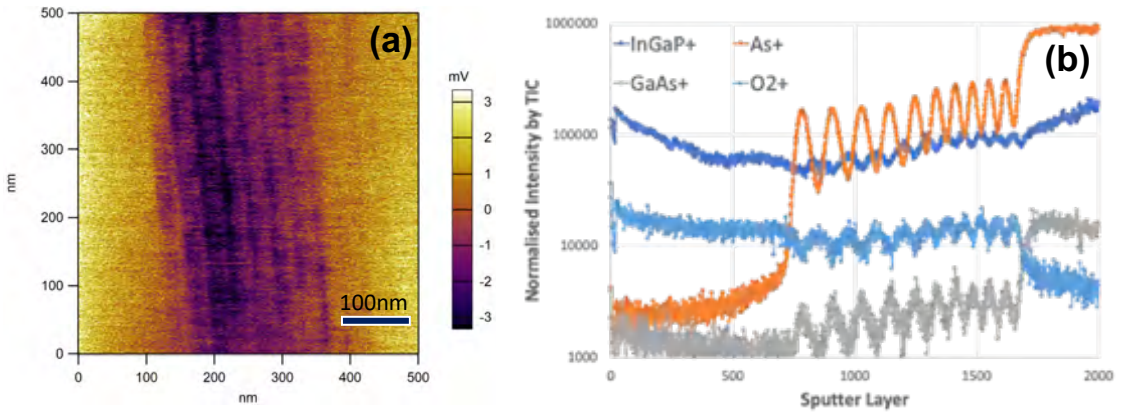


Figure 1. a) Conductance image showing the depth profile exhibiting contrast arising from the materials with different band gaps. The conductance is shown in a reverse falso color table, with dark meaning higher conductance and bright lower conductance. b) Depth profile of the same stack, exhibiting the composition modulation consistent with the nominal structure.

[1] Ohlberg, D.A.A.,. *et al*. The limits of near field immersion microwave microscopy evaluated by imaging bilayer graphene moiré patterns. Nat Commun 12, 2980 (2021)

Quadrupole SIMS for SiGe Process Control:

Low-Energy Depth Profiling and Quantification

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Silicon–germanium (SiGe) heterostructures are widely used in advanced CMOS and RF technologies, where device performance depends critically on germanium concentration, dopant distribution, and interface abruptness. As SiGe layers become thinner and composition gradients steeper, reliable and quantitative depth profiling with high depth resolution and repeatability remains a significant metrology challenge.

In this work, SiGe structures are characterized by dynamic SIMS using a quadrupole mass analyzer on the CAMECA SIMS 4550 platform. Low-impact-energy oxygen sputtering at normal incidence is employed as the primary analytical protocol, enabling stable sputtering conditions and optimized depth resolution [1]. Optical Conductivity Enhancement (OCE) is used to mitigate charging effects in low-conductivity or strained SiGe layers, ensuring stable secondary-ion signals and improved measurement repeatability.

Representative depth profiles of Si, Ge, and boron are presented. The influence of analytical parameters, including primary ion species, impact energy, and incidence angle, is discussed with respect to depth resolution, erosion rate, and signal stability. Using oxygen-based protocols, germanium quantification is achieved through direct $Si_{1-x}Ge_x$ normalization, taking advantage of relative sensitivity factors that remain constant over a wide range of Ge concentrations. The variation of erosion rate with Ge content is accounted for to obtain accurate depth scaling in graded structures. Boron quantification is shown to be weakly dependent on Ge concentration, enabling reliable dopant profiling across SiGe ramps.

Excellent same-day and day-to-day repeatability is demonstrated for both Ge concentration (sub-percent relative variation) and dopant depth positioning (sub-nanometer), highlighting the robustness of the approach. These results demonstrate that low-energy quadrupole SIMS operated with optimized oxygen sputtering and charge compensation provides a reliable and quantitative solution for SiGe depth profiling, supporting both research characterization and semiconductor process control.

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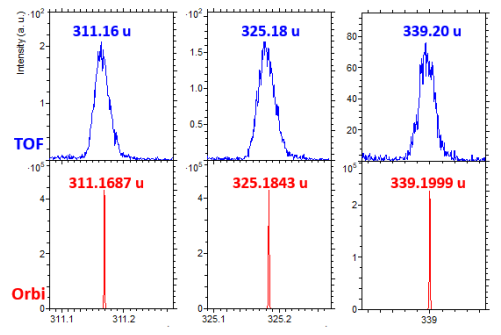
Applications of Orbitrap-SIMS in Failure Analysis of LCD Panels

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Failure analysis (FA) of liquid crystal display (LCD) panels critically relies on the precise identification of surface contaminants. TOF-SIMS is a widely used surface analysis technique with excellent sensitivity for characterizing inorganic species (e.g., Na^+ and K^+). However, the accurate identification of unknown contaminants in the high mass range (m/z > 200) remains a major technical challenge.

In light of this limitation, Orbitrap-SIMS delivers up to a ~20-fold improvement in mass resolution compared to TOF-SIMS, while achieving a mass accuracy of below 1 ppm [1,2]. To confirm its analytical capability, the panel surface was deliberately contacted with cleanroom-grade examination gloves, simulating contamination by several unidentified components (m/z = 311, 325, 339). While TOF-SIMS offers limited mass resolution, Orbitrap-SIMS provides the accurate mass necessary to elucidate chemical composition (Fig. 1). Further MS/MS analysis via Orbitrap-SIMS enabled the identification of key fragment ions such as SO_3^- and $C_8H_7SO_3^-$, allowing the deduction that these components are alkyl-substituted benzenesulfonate derivatives. Beyond lab simulations, aluminum-oxygen (Al-O) clusters were detected in an actual FA case. It was further observed that different primary ion sources yield distinct secondary ions from Al-O cluster; specifically, the Bi-source generates more fragments in the higher mass range (m/z > 1000) compared to GCIB-source (Fig. 2). Qualitative identification of other unknown contaminants was further performed across other cases, collectively demonstrating the broad application prospects of Orbitrap-SIMS in FA of LCD panels.



Mass (u)	Assignment	Deviation (ppm)
311.1687	C_17H_27SO_3-	0.233
325.1843	C_18H_29SO_3-	0.043
339.1999	C_19H_31SO_3-	-0.140

Figure 1. Mass resolution: Orbitrap vs. TOF

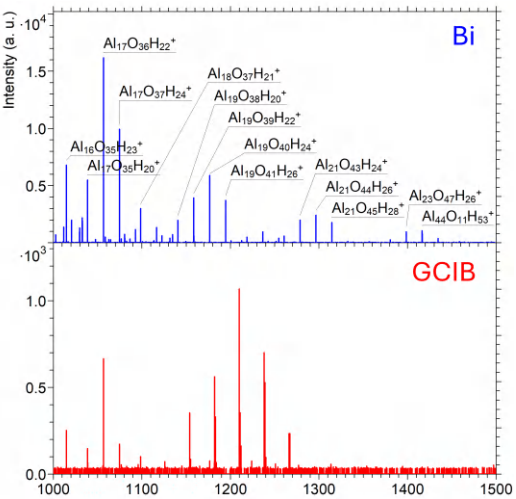


Figure 2. Primary ion: Bi vs. GCIB

Reference:
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Studies and Applications of TOF-SIMS in F-induced Corrosion Defect Characterization

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In modern semiconductor manufacturing, defect characterization plays a critical role in improving product yield and reliability. Time-of-Flight Secondary Ion Mass Spectrometry (TOF-SIMS) has emerged as a powerful analytical technique for surface and defect analysis due to its ultra-high sensitivity, high mass resolution, and capability to detect all elements including hydrogen and its isotopes. This paper presents a comprehensive study on the application of TOF-SIMS in F-induced corrosion defect characterization on aluminum bondpads in wafer fabrication. TOF-SIMS offers several unique advantages, including a detection limit down to the ppm-ppb level and the ability to simultaneously acquire spectral, imaging, and depth profiling information. These capabilities make it an indispensable tool for identifying trace-level contaminants and understanding failure mechanisms at the nanoscale.

In this paper, TOF-SIMS was employed to investigate abnormal aluminum bondpads exhibiting non-stick bond pad (NSOP) issues. Optical microscopy and SEM inspection revealed "flower-like" defects on the affected bondpads, while EDX and XPS analyses detected high levels of fluorine contamination. XPS further identified an unknown Al-F compound with a binding energy of 78.7 eV. To identify this unknown compound, TOF-SIMS analysis was performed. The results showed significantly elevated ion counts of $[AlF_4]^-$ on defective bondpads compared to normal pads. Based on the chemical stability constants ($K_{Total} = 6.92 \times 10^{19}$) and the hexagonal morphology observed by SEM, the unknown compound was identified as aluminum hexafluoride, $[AlF_6]^{3-}$. This finding is further supported by electrochemical theory, where the highly negative standard electrode potential ($E° = -2.07$ V) favours the formation of $[AlF_6]^{3-}$ in the presence of fluorine contamination. Furthermore, a theoretical corrosion model was established, demonstrating that fluorine-induced corrosion is enhanced by water vapor and oxygen.

In conclusion, TOF-SIMS proves to be an invaluable technique for defect characterization, enabling the identification of complex chemical species and providing critical insights into corrosion mechanisms. This study not only contributes to the understanding of fluorine-induced corrosion but also offers practical guidance for quality control in semiconductor manufacturing.

Keywords : TOF-SIMS, XPS, Al Bondpads, F-induced Corrosion, Defect Characterization.

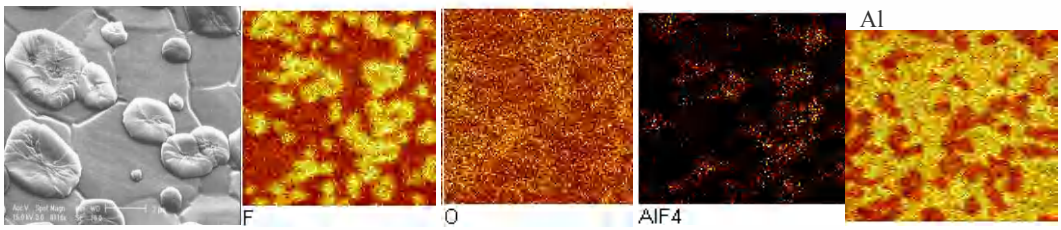


Fig.1. SEM photo of the defects and the detection of $[AlF_4]^-$ ions by TOF-SIMS ion mapping confirms the presence of $[AlF_6]^{3-}$.

Mass Spectroscopic Characterization of the Photoresist Post Exposure Process

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Mass spectroscopic investigation of the photoresist exposure process plays a crucial role in elucidating the underlying reaction chemistry and provides valuable guidance for material selection and process optimization. In this study of photoresist behavior after exposure, several distinct mass peaks—particularly in the range of 150–350 amu—are observed during the exposure process. These peaks are attributed to molecular chain scission of the photoresist matrix or its additives, induced by photoacid generator (PAG)–derived acid attack during exposure. Figure 1 illustrates representative examples of these distinct mass peaks.

Monitoring the emergence and evolution of these mass peaks after exposure enables insight not only into the static chemical composition but also into the dynamic chemical transformations that facilitate lithographic pattern formation. The increase in intensity—and in some cases the exclusive appearance—of these peaks serves as a direct spectroscopic signature of the acid-catalyzed deprotection reaction in progress. Consequently, these peaks represent valuable process monitors for (1) photoresist sensitivity, (2) acid diffusion behavior, (3) reaction completeness, and (4) process window characterization. Importantly, the progressive increase in peak intensity, rather than mere peak appearance, provides quantitative information on reaction kinetics and overall process efficiency.

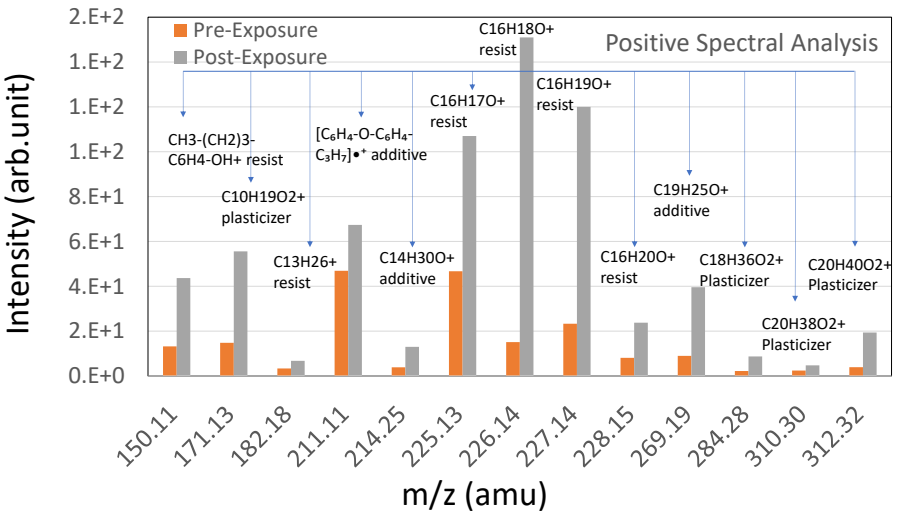


Figure 1. Some of the signature mass peaks assigned from the photoresist for post exposure versus pre exposure

Magnetic Sector Dynamic SIMS for Complex Structures and High-Resolution Depth Profiling

AS. Robbes[1], P. Peres[1], S. Choi[1], K. Soulard[1], J. Ren[1], B. Sallé[1], M. Haberbusch[1], J. Araujo[1], O. Dulac[1], T. Faye[1], J. Bai[2], A. Zou[2]

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Dynamic Secondary Ion Mass Spectrometry (Dynamic SIMS) remains a reference technique for quantitative, depth-resolved analysis of advanced materials, offering unparalleled sensitivity for trace-level detection. Current and emerging challenges, particularly in semiconductor and functional materials, are driven by increasingly complex structures combining thick stacks, deeply buried features, and critical thin layers requiring precise depth control.

In this oral contribution, the authors present recent advances in magnetic sector Dynamic SIMS instrument architecture aimed at addressing these evolving analytical requirements. The work focuses on improving analytical performance across different dynamic SIMS regimes, enabling depth profiling strategies adapted to a broad range of material systems.

A central aspect of these developments is the ability to investigate extended structures, allowing Dynamic SIMS to address different applications ranging from profiling of thick structures to high-resolution analysis of thin layers. Operation at reduced sputtering energies is particularly important to limit ion-induced mixing and improving depth resolution. These developments enhance sensitivity and detection limits for trace elements, including atmospheric species, thereby increasing quantitative reliability in depth profiling experiments.

Advances in instrument automation are also presented, addressing operational complexity and usability. Automated alignment minimizes operator-dependent variability, shortens setup time, and directly supports higher analytical throughput and reproducibility.

Representative application examples illustrate how these combined advances enable Dynamic SIMS measurements of complex structures, demonstrating how modern magnetic sector Dynamic SIMS can meet current and future analytical demands in both research and industrial environments.

Evaluating the influence of lipid nanoparticles on macrophages using OrbiSIMS and machine learning

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Lipid nanoparticles (LNPs) are important materials in the medical field, and their functions strongly depend on their surface and internal structures and states. In particular, polyethylene glycol (PEG), which is used to modify the nanoparticle surface, contributes to particle stabilization. However, its potential effects on immune responses have raised concerns, and the need to investigate alternative materials has recently increased. Against this background, it is important to evaluate in detail the distribution and chemical states of surface-modifying molecules, as well as their interactions with biological cells and tissues. Although secondary ion mass spectrometry (SIMS), which provides detailed chemical information and a two-dimensional (2D) spatial resolution of approximately 100 nm for organic materials, is one of the most effective methods to evaluate such nanoparticles, it does not have high enough resolution for imaging nanoparticles in terms of 2D imaging. In contrast, in depth profiling analysis, high depth resolution on the order of several nanometers can be achieved by using gas cluster ion beams (GCIBs), such as Ar cluster ion beams. The objectives of this study are, therefore, to evaluate cell membranes treated with nanoparticles and the structures of the nanoparticles by depth profiling using GCIBs as both the primary ion and as the sputtering ion beams. In addition, OrbiSIMS, a time-of-flight secondary ion mass spectrometry (ToF-SIMS) equipped with an Orbitrap mass analyzer with high mass-resolving power (approximately 240,000 at m/z 200), was employed to identify mass peaks derived from biomolecules. Three types of PEG-modified lipid nanoparticles with different diameters and different PEG concentrations were used as model samples. Macrophages were exposed to each LNP sample for 0, 2, 4, or 8 hours before the OrbiSIMS measurement. This allowed us to evaluate the effects of particle size and PEG concentration on the time-dependent changes in macrophage-derived secreted substances. However, the biological samples such as those investigated in this study contain many unknown and complex peaks, and the data obtained by OrbiSIMS are extremely large numbers of variables (mass peaks). Therefore, unsupervised machine learning methods, including principal component analysis (PCA), multivariate curve resolution (MCR), and sparse autoencoder (SAE) and supervised machine learning methods, were used to classify and interpret the SIMS data according to their features. Furthermore, to identify factors more specifically associated with particular samples or conditions, the supervised machine learning method random forest was applied to predict the type of each sample dataset and to extract important peaks for the target samples and conditions. As a result, the chemical composition of the LNP-treated macrophage samples and differences in preparation conditions, such as particle size and PEG concentration, as well as depth-dependent changes from the surface to internal, were indicated.

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[3] S. Aoyagi et al., Analytical Chemistry, 93, 9, 4191-4197 (2021).

Spatially-Informed Multi-Omics Analysis of Parkinsonian Circuits: A ToF-SIMS-Based Proteomic Investigation

Sun Young Lee[1], Hyun Kyong Shon[1], Amos Chungwon Lee[2], Kyoung-Shim Kim[3], Sunghoon Kwon[2], Jeong Hee Moon[4], Tae Geol Lee[1,*], Jin Gyeong Son[1,*]

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(2)Bio-MAX Institute, Seoul National University, Seoul 08826, Republic of Korea
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The spatial heterogeneity of metabolic and proteomic alterations in neurodegenerative diseases remains insufficiently resolved, necessitating analytical approaches that preserve anatomical context . We present a high-resolution, multilayered analytical framework that anchors time-of-flight secondary ion mass spectrometry (ToF-SIMS) within a spatially guided multi-omics workflow to interrogate the 6-hydroxydopamine (6-OHDA) mouse model of Parkinson's disease.

Our strategy leverages the superior spatial sensitivity of ToF-SIMS to identify region-specific molecular asymmetry, which subsequently informs the precise isolation of microenvironments for deep proteomic profiling via laser cell sorting. In the substantia nigra, the primary lesion site, ToF-SIMS imaging revealed a distinct lipid signature defined by monounsaturated fatty acid enrichment and selective phospholipid remodeling (PS 36:1, PI 36:3/36:1). This spatial lipidomic profile was functionally coupled with proteomic downregulation of mitochondrial oxidative phosphorylation, confirming a localized metabolic-proteomic convergence.

Importantly, this ToF-SIMS-anchored approach uncovered a pathological continuum extending beyond the primary nigrostriatal axis. While lipid remodeling was concentrated in the lesion core, distal projection areas such as the hippocampus and piriform cortex exhibited large-scale proteomic adaptations involving synaptic vesicle cycles and intracellular transport. These findings demonstrate that our integrative MSI-proteomics platform can delineate both primary neurochemical stress and secondary circuit-level adaptations, providing a foundation for future spatially-resolved investigations into neurodegenerative progression.

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Comparison of difference in OrbiSIMS spectra of macrophages caused by sample preparation using machine learning

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Time-of-flight secondary ion mass spectrometry with Orbitrap (OrbiSIMS)[1,2] is a powerful technique for biological analysis, providing label-free molecular-level mass and spatial information by bombarding samples with a primary ion beam under ultra-high vacuum ($<10^{-8}$ mbar) and analysing the resulting secondary ions. However, measuring biological samples with high water content under such ultra-high vacuum conditions, whilst retaining as much information as possible, requires an appropriate preprocessing method. Freeze-drying, in which water is removed by sublimation after freezing, and frozen hydration, in which water is retained in an amorphous state at extremely low temperatures, have been investigated [3,4]. In this study, macrophage samples were prepared using three different preprocessing methods and analysed using OrbiSIMS depth profiling, and the resulting depth profiles were then compared. Specifically, samples in a frozen-hydrated state, samples freeze-dried in situ within the OrbiSIMS instrument by gradual warming from −170 °C to room temperature, and samples subjected to conventional freeze-drying outside the instrument were analysed. Furthermore, unsupervised machine learning methods, including principal component analysis and multivariate curve resolution, were applied to OrbiSIMS spectra to obtain an overview of the data [5] and to classify important features. Additionally, a supervised machine learning method, such as random forest [5-7], was applied to extract specific mass peaks associated with a particular sample.

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Organic–Halogen Induced Corrosion of Cu Bond Pads Revealed by TOF-SIMS

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Abnormal discoloration of Cu bond pads—showing a reddish center relative to the edge—was investigated by Auger electron spectroscopy (AES) and time-of-flight secondary ion mass spectrometry (TOF-SIMS) in both positive and negative ion modes. AES revealed pronounced Cl enrichment at the pad center, while TOF-SIMS resolved significant spatial variations in organic and inorganic species. In positive ion mode, the center region showed elevated hydrocarbon ($C_xH_y^+$), oxygenated ($C_xH_yO^+$), and nitrogen-containing ($C_xH_yN^+$) fragments, together with Cu-related species ($CuOH_2^+$, Cu_2OH^+, and Cu–organic complexes), indicating the co-existence of organic residues and enhanced Cu surface oxidation.

Complementary negative ion spectra showed enhanced signals from halogen-related species (Cl^-, F^-, C_2HCl^-, C_2HOCl^-), oxidized Cu clusters (CuO_2^-, $Cu_3O_3^-$), and hybrid ions containing Cu, O, N, and halogens (e.g., $CuClO^-$, $CuOF^-$, C_2NOCuF^-). Their concurrent enhancement at the center points to the formation of Cu–organic–halogen complexes within a chemically heterogeneous surface environment.

The discoloration is therefore attributed to localized under-film electrochemical corrosion driven by the synergistic action of organic residues and halogen contaminants: hygroscopic organic layers promote moisture adsorption and electrolyte formation, while halide species destabilize the native oxide and promote Cu dissolution followed by re-oxidation to Cu_2O, producing the observed reddish appearance. This work demonstrates that combined positive/negative TOF-SIMS analysis can resolve complex corrosion chemistries and provides mechanistic insight into contamination-induced degradation of Cu surfaces.

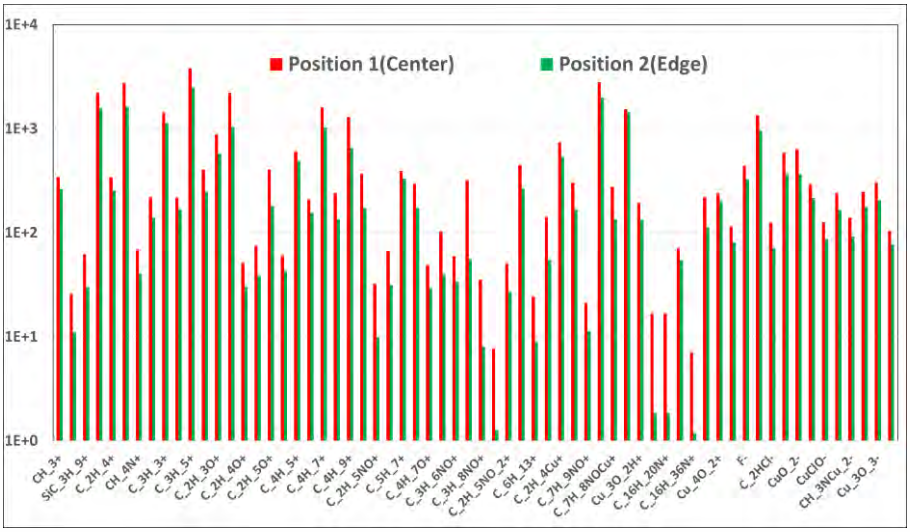


Figure 1 Bar chart of TOFSIMS fragment ions

Ultra-Thin Oxynitride Gate Dielectric Characterization by Dynamic SIMS at Ultra-Low Impact Energy

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Ultra-thin silicon oxynitride (SiON) layers remain a key dielectric material in advanced CMOS technologies, where nitrogen dose, depth distribution, and interfacial abruptness critically impact device performance and reliability. As equivalent oxide thicknesses scale to a few nanometers, accurate characterization of nitrogen in SiON structures becomes increasingly challenging due to the extremely shallow profiles involved and the need for high sensitivity combined with excellent depth resolution.

Dynamic SIMS operated under ultra-low impact energy conditions provides a powerful metrology solution for these applications, enabling reliable depth profiling of ultra-thin dielectric layers while preserving dynamic range. The combination of low energy Cs^+ sputtering, high secondary ion transmission, and magnetic sector mass analysis is particularly well suited for resolving nitrogen, oxygen, and silicon in-depth distributions in SiON gate stacks.

In this contribution, we present representative oxynitride characterization results obtained using the CAMECA IMS Wf and SC Ultra magnetic-sector SIMS instruments. Two analytical conditions are compared in terms of nitrogen depth resolution, profile shape fidelity, signal stability, and suitability for routine versus very-shallow measurements. The influence of grazing incidence and analytical configuration on nitrogen profiling in SiON gate stacks is discussed, together with implications for repeatability and process monitoring.

These results illustrate how the flexibility of ultra-low energy dynamic SIMS enables optimization of analytical conditions for quantitative characterization of advanced oxynitride gate dielectrics.

Identification and degradation evaluation of ocean plastic pieces using imaging techniques and machine learning

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Ocean plastic is one of the most significant global environmental issues [1] due to its impact on ecological systems including human health. Plastic is widely used because it is inexpensive to produce and highly durable; this also means that it is not easily biodegradable. Once plastic products enter the ocean, they are degraded into micro-size pieces and remain in the ocean for an extremely long time. For example, plastic products in the ocean are broken down by ultraviolet rays and waves into fragments known as microplastics. To address the ocean plastic problem, it is necessary to understand how plastic products degrade into microplastics, specifically by elucidating the degradation processes of plastics. To evaluate the degradation of plastics collected from marine environments, each plastic fragment must first be identified and classified. Furthermore, interest in plastic recycling technologies has increased in recent years. The identification of unknown plastics is also essential for effective recycling. Identifying completely unknown plastic pieces, such as ocean plastic, can be difficult using time-of-flight secondary ion mass spectrometry (ToF-SIMS) or OrbiSIMS, particularly when the molecular weight of the plastic is higher than the SIMS mass range. In this study, two white plastic samples of different sizes were analysed using Raman spectroscopy to classify the type of plastic and OrbiSIMS to evaluate the chemical conditions at each depth. Raman spectroscopy was employed to classify the type of plastic. Kendrick mass defect (KMD) analysis was then applied to the SIMS spectra to identify the monomers of the plastic. Moreover, the degradation of the ocean plastic pieces was evaluated by analysing the depth profiles obtained with OrbiSIMS using machine learning techniques [2,3]. Degradation was evaluated by comparing the surface of the ocean plastics, which is more significantly affected by degradation and contamination, with the interior, which is less affected and retains the original plastic structure [4].

The authors thank Prof. Atsuhiko Isobe for generously providing ocean plastic samples.

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Single-Cell Metabolic Imaging of the Tumor Microenvironment Using ToF-SIMS

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Elucidating metabolic heterogeneity within the tumor microenvironment (TME) at single-cell resolution is important for understanding hepatocellular carcinoma (HCC) progression. However, current imaging methods often face a trade-off between spatial resolution and reliable metabolic information.

In this work, a label-free workflow based on time-of-flight secondary ion mass spectrometry (ToF-SIMS) is developed for single-cell metabolic imaging of mouse HCC tissues. The workflow combines optimized sample preparation with high-throughput spatial single nuclEar metAboloMics (SEAM), aiming to improve both data reliability and single-cell analysis [1-2].

Different sample pretreatment methods are systematically compared, and freeze-drying is identified as the most suitable approach. It preserves tissue structure and metabolite signals while reducing molecular movement and signal loss. The SEAM method is further improved to increase its speed and stability when processing large-area ToF-SIMS data, enabling automatic single-cell segmentation and metabolic analysis directly from imaging data.

This workflow enables mapping of metabolic differences across the tumor microenvironment at single-cell resolution. Distinct metabolite distributions and spatial organization patterns are observed among different cell groups.

Overall, this work provides a reliable and scalable method for single-cell spatial metabolomics and offers a useful tool for studying metabolic heterogeneity in complex tumor tissues.

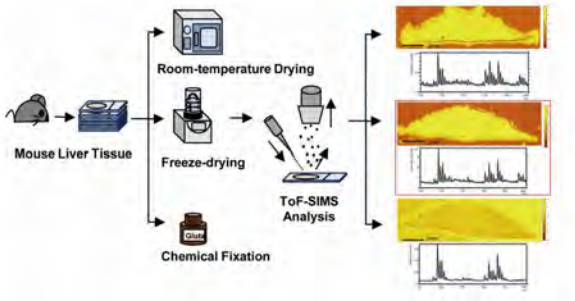


Figure 1. Optimized freeze-drying enables ToF-SIMS to preserve tissue structure and lipid signals, improving molecular imaging of biological samples.

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ToF-SIMS Tracking of Thermal Reorganization in ODPA Inhibitor Layers on GaN

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Abastract: Self-assembled monolayers (SAMs) tailor surface chemistry and can serve as inhibitor layers for area-selective atomic layer deposition (AS-ALD). Their inhibition performance depends on thermal stability and interfacial bonding under ALD-relevant heating. This makes surface-sensitive chemical analysis important for understanding their evolution on compound semiconductor surfaces. Here, time-of-flight secondary ion mass spectrometry (ToF-SIMS) was used to examine microcontact-printed octadecylphosphonic acid (ODPA) layers on GaN after annealing from room temperature to 200 °C. Selected negative-ion fragments were tracked to evaluate the thermal reorganization of ODPA on GaN (Figure 1). As the annealing temperature increased, the substrate-derived $^{71}Ga^{14}N^-$ signal increased, whereas PO_3^-, $[ODPA–H]^-$, and $[ODPA_2–H]^-$ decreased. These trends indicate loss and restructuring of loosely bound ODPA species, which reduces attenuation of substrate-related secondary ions. In parallel, $^{69}GaOP^-$ and $[ODPA_2–H_2O–H]^-$ increased, consistent with thermally promoted interfacial condensation and intermolecular reorganization. These results suggest that annealing converts part of the printed ODPA layer into a more reorganized and interfacially anchored inhibitor layer. This study shows that ToF-SIMS can resolve molecular-level changes in printed SAM inhibitors and provides chemical insight into thermally stable molecular templates for selective dielectric growth on GaN.

Keywords: ToF-SIMS; ODPA; GaN; Thermal reorganization; Interface chemistry

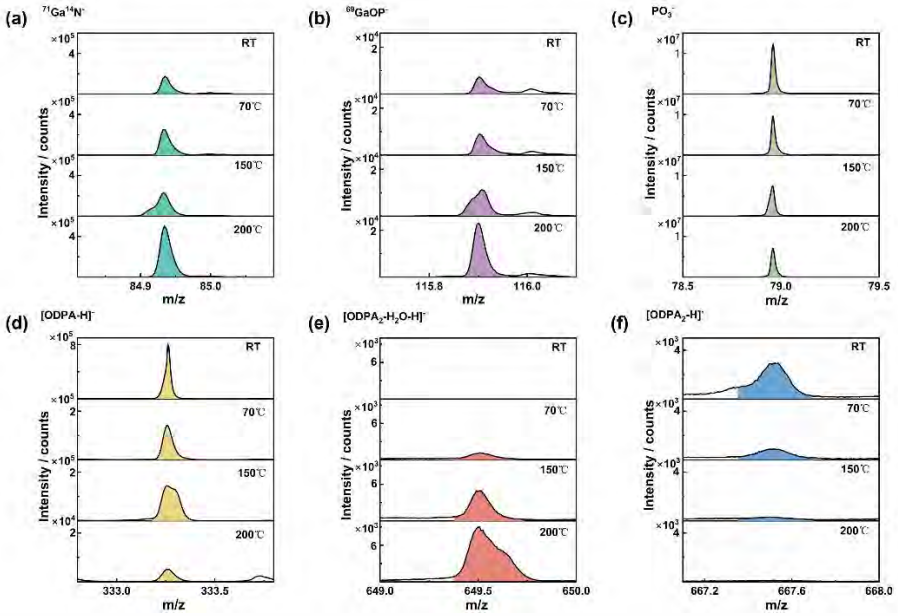


Figure 1. Temperature-dependent negative-ion ToF-SIMS spectra of ODPA-covered GaN after annealing from room temperature to 200 °C.

Non-canonical autophagy restores lipid nanoparticle-mediated inflammation and toxicity

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Lipid nanoparticles (LNPs) have emerged as the leading non-viral platform for the intracellular delivery of nucleic acid-based therapeutics, achieving landmark clinical approvals for small interfering RNA (siRNA) delivery and mRNA-based vaccines against SARS-CoV-2. Despite their therapeutic potential, widespread clinical use is limited by their tendency to elicit inflammatory responses[1].

Ionizable lipids have been proposed as the primary drivers of LNP-induced inflammatory responses[2]. Understanding how cells sense, process, and respond to ionizable lipids at the subcellular level is therefore a prerequisite for the rational design of safer and more effective LNP systems. A major impediment has been the lack of analytical tools capable of visualizing the nanoscale subcellular localization of ionizable lipids with sufficient spatial resolution and chemical specificity.

Here, employing NanoSIMS imaging of deuterium-labeled ionizable lipids, we reveal for the first time the subcellular distribution of ionizable lipids in cells and tissues. Unexpectedly, the majority of ionizable lipids are retained within the endolysosomal compartments despite evident membrane damage. This retention triggers calcium-dependent, noncanonical conjugation of ATG8/LC3B to lysosomal membranes (CASM), independently of canonical autophagy[3]. This Ca^{2+}-leakage-dependent non-canonical autophagy pathway facilitates lysosomal membrane repair, ionizable lipid clearance, and restriction of LNP-associated cytotoxicity and inflammatory signaling, defining a previously unrecognized quality-control axis at the LNP-lysosome interface. and layout for individual paragraphs.

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ToF-SIMS Study on the Interfacial Structure and Formation Mechanism of Black Decorative Layer of Cizhou Kiln White-Ground Black-flower Porcelain

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Cizhou Kiln white-ground black-flower porcalain is a quintessential representative of Northern Chinese ceramic art, characterized by a stratified microstructure comprising a ceramic body, white slip, black pigment layer, and a transparent glaze. The aesthetic quality of this ware is fundamentally determined by the interplay of these layers, where the opacity of the slip, the chromatic properties of the pigment, and interfacial reactions are critical to elucidating ancient manufacturing technologies.

While this decorative technique flourished during the Song Dynasty, the Ming Dynasty witnessed significant evolution and inheritance of these traditions. This study employs Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) to conduct high-spatial-resolution elemental mapping on cross-sections of Song and Ming dynasty samples. By focusing on chromophoric elements (Fe, Mn) and matrix constituents (Si, Al, Ca, K, Na), we investigate the distribution profiles, diffusion mechanisms, and interlayer differentiation across different historical periods.

The ToF-SIMS characterization elucidates the precise composition of the black decorative layer, its coloration mechanism, and the complex interactions at material interfaces. These findings provide novel material evidence for the technological history of Cizhou Kiln and demonstrate the immense potential of ToF-SIMS in the microanalytical investigation of ancient ceramic interfaces.

Keywords:

Cizhou Kiln; ancient ceramic; white-ground black-flower porcalain; ToF-SIMS; interfacial structure

Direct visualization of APP on lipid rafts using time-of-flight secondary ion mass spectrometry

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Lipid rafts within the plasma membrane are known to act as dynamic signaling hubs by clustering proteins involved in common pathways. However, the lack of direct and simultaneous visualization of lipid rafts and associated proteins has limited our understanding of their functional roles in diverse biological contexts. In Alzheimer's disease (AD), amyloid-β (Aβ) is produced from sequential cleavage of amyloid precursor protein (APP) by β- and γ-secretases, predominantly in endosomes following APP internalization via clathrin-mediated endocytosis. In this study, we established a novel imaging protocol utilizing time-of-flight secondary ion mass spectrometry (ToF-SIMS) to directly observe APP localization on lipid rafts. Using this approach, we discovered that astrocyte-derived ApoE4 enhances the association of APP with lipid rafts, which in turn increases $A\beta_{42}$ production through a clathrin-independent mechanism in neurons.

Highly site-selective fragmentation of peptides induced by MeV-ion impact

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Secondary ion mass spectrometry based on high energy ions in the MeV energy range is seen as an alternative for soft SIMS analysis of organic material. In order to better understand the excitation mechanisms operative in MeV-SIMS, we investigated the fragmentation of oligopeptides induced by swift heavy ions (SHI, Fig. 1(a)). For the analysis of the SHI-induced fragments, we made use of soft desorption/ionization induced by neutral SO_2 clusters (DINeC) in combination with mass spectrometry (Fig. 1(b)). With their different functional groups and bonds, peptides are an ideal model system to investigate the interaction of SHI with organic molecules. Furthermore, peptides represent one of the most important classes of biomolecules; therefore, their interaction with SHI is also of interest, e.g., for medical applications.

Our experimental results clearly indicate that, despite the high initial energy deposition, SHI-induced peptide fragmentation is highly site-selective with respect to the position of the cleavage site in the amino acid sequence (Figs. 1(c)-(e)). We could further show that the amino acids in the direct neighborhood of the cleavage sites do *not* determine the site selectivity, in contrast to low-energy dissociation processes. The observed selectivity rather depends on the whole structure of the peptide.

Ab initio molecular dynamics calculations suggest multiple electron abstraction as a possible excitation process for SHI-induced peptide fragmentation and the observed site selectivity. Together with the experimental results, they point towards a unique excitation channel operative under swift heavy ion impact which will also govern the sputter process in MeV-SIMS.

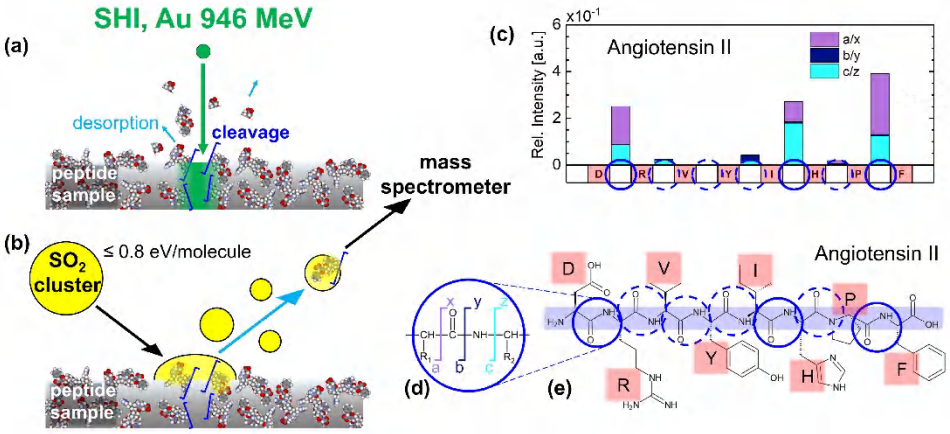


Fig. 1: (a) and (b) Fragmentation induced by SHI is analyzed by DINeC-MS. (c) to (e) The resulting distributions of fragments show high site-selectivity with respect to the cleavage site in the peptide.

ToF-SIMS Depth Profiling of Dielectric/Metal/Dielectric Multilayers for Spectrally Selectivity in Semi-transparent Perovskite Solar Cells

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Dielectric/metal/dielectric (D/M/D) multilayers represent a class of nanoscale-engineered architectures where an ultrathin metallic layer is sandwiched between two dielectric films to simultaneously optimize optical transmission and electrical conductivity. In this study, we present the fabrication and characterization of symmetric and asymmetric D/M/D structures based on ultrathin metal films and molybdenum/tungsten oxide (MoO_3, WO_3) dielectric layers. These architectures are designed to enable spectral selectivity in the visible and near-infrared regions, a crucial feature for their integration as transparent top electrodes in semi-transparent perovskite solar cells.

To this end, the nanoscale structure and the elemental distribution within the D/M/D stacks were investigated by means of Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS). By utilizing high-resolution depth profiling, we monitored the distribution of Au, Mo, and W species through the multilayer, assessing the sharpness of the interfaces and the absence of elemental diffusion, which is critical for maintaining spectral selectivity without compromising electrical performance.

This ToF-SIMS analysis, integrated within a multi-technique approach including XPS, AFM, and UV–Vis–NIR spectroscopy, allowed to correlate the stacking sequence with the observed optoelectronic properties. The results demonstrate how the assessment of the chemical and structural integrity at the nanoscale ensures the stability required for high-efficiency, tunable transparent electrodes in next-generation photovoltaics.

Advanced SIMS-Based Methodology for Dopant Depth Profiling and Quantification in 4H-SiC

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4H-SiC (4H-Silicon Carbide) is a semiconductor material characterized by high thermal stability, a wide bandgap, and strong potential for high-power and high-temperature electronic devices, which has attracted significant attention in recent years. Ion implantation is the most widely used technique for introducing dopants into 4H-SiC; however, it induces significant lattice damage and requires high-temperature annealing processes to restore crystal order and activate the dopants.

During ion implantation and subsequent diffusion processes, accurate control of dopant depth profiles in silicon carbide remains a critical challenge, with additional complexities compared to conventional semiconductors. As a consequence, advanced and dedicated analytical approaches are still required and represent an active field of investigation.

In this work, a comprehensive and methodological analytical approach based on secondary ion mass spectrometry (SIMS) is presented for the investigation of doped SiC samples. Particular attention is devoted to the characterization of dopant depth profiles, as well as to the optimization of analysis and quantification procedures in order to achieve reliable and accurate profiling.

Dynamic SIMS is employed to obtain quantitative depth distributions of dopants, while TOF-SIMS provides complementary information on near-surface chemistry and potential redistribution effects. In addition, AFM analyses are carried out to assess morphology evolution induced by implantation and thermal treatments, enabling correlation between chemical profiles and surface modifications.

The developed analytical framework is applied to dopant profiles obtained after implantation at different doses and energies, followed by annealing treatments in the range of 1650–1850 °C for durations between 20 and 60 minutes. The results provide relevant insights into the mechanisms governing dopant behavior in wide-bandgap semiconductors and support the optimization of implantation and annealing processes for advanced SiC device fabrication.

More broadly, this study highlights SIMS as a key enabling technique for the characterization of emerging microelectronic materials and underlines the need for the development of dedicated analytical methodologies tailored to wide-bandgap semiconductor systems.

Tracing the Technological Transition of Chinese Blue-and-White Porcelain: A ToF-SIMS Study of Body-Glaze Interfacial Reactions and Cobalt Migration

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The origin and maturation of Chinese blue-and-white porcelain are reflected not only in vessel forms and decorative styles, but also in high-temperature interactions among the ceramic body, glaze, and cobalt pigment. Tang–Song blue-and-white porcelain from the Yingou site and Yuan blue-and-white porcelain from Jingdezhen represent the early exploratory and mature production stages, respectively. Their body-glaze interfaces and blue decorative layers provide important evidence for investigating the technological evolution of blue-and-white porcelain. However, systematic comparative studies on body-glaze interfacial reactions and cobalt migration behavior at the microscale remain limited. In particular, the development of interfacial reaction layers, directions of elemental diffusion, distribution of cobalt within the glaze, and spatial coupling of chromophoric and associated elements such as Co, Fe, and Mn remain insufficiently understood.

In this study, Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) will be used to conduct high-spatial-resolution elemental imaging and depth-profile analysis of the body, glaze, and body-glaze interface in the two groups of samples. Concentration gradients of matrix elements, including Si, Al, K, Na, and Ca, will be compared to evaluate interfacial reaction layer development and elemental exchange. The enrichment patterns, migration depths, and spatial associations of Co, Fe, and Mn in the blue decorative regions will also be examined. By comparing interfacial continuity, elemental diffusion, and microscale heterogeneity between the two groups, this study aims to identify key technological changes from early experimentation to mature production.

This study is expected to provide microscopic material evidence for understanding the technological evolution from early to mature blue-and-white porcelain from the perspective of interactions among the ceramic body, glaze, and cobalt pigment.

Keywords: Blue-and-white porcelain; ToF-SIMS; elemental migration; cobalt migration; interfacial reaction

Characterization of Hydrogen Distribution in Power Semiconductor Materials

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Power semiconductor devices are required to ensure operational stability in high-voltage and high-temperature environments. Conventional silicon (Si) is fundamentally limited by its narrow bandgap (1.12 eV), which leads to uncontrollable leakage currents driven by thermal excitation during high-temperature operation. In contrast, prominent Wide Bandgap (WBG) semiconductors, such as silicon carbide (SiC, Eg ≈ 3.26 eV) and gallium nitride (GaN, Eg ≈3.4 eV) exhibit high critical breakdown field, enabling a significant reduction in device active layer thickness for a given breakdown voltage rating. Additionally, the superior thermal conductivity of SiC enables efficient heat dissipation, while the high electron mobility of GaN optimizes high-frequency switching performance. However, the fabrication of WBG power semiconductor devices frequently introduces hydrogen species, which result in defect formation, lattice strain, and increased leakage current that exhibit distinct behaviors by different material matrices. Therefore, analytical techniques optimized for precisely quantifying hydrogen ion concentrations within specific substrates are critical. Secondary Ion Mass Spectrometry (SIMS) is the most powerful technique for the quantitative analysis of trace hydrogen due to its exceptional sensitivity and depth resolution [1].
In this study, hydrogen ions were irradiated into three representative power semiconductor matrices (Si, SiC, and GaN) using a gas ion implanter. Using M-SIMS, we precisely characterized the depth profiles, accounting for the distinct atomic densities and stopping powers of each substrate. This research demonstrates how hydrogen ion distribution behaviors vary depending on the substrate matrix, through a comparative quantitative analysis of projected range and concentration, providing essential data for advanced power device engineering.

Acknowledgement
This research was supported by the Korea Industrial Technology Association (KOITA) grant funded by the Korea government (Ministry of Science and ICT) (2710093406). Gas ion implanter was supported by the KOMAC (Korea Multi-purpose Accelerator Complex) operation fund of KAERI (Korea Atomic Energy Research Institute)

Keywords: Power Semiconductor, SiC, GaN, Hydrogen, M-SIMS, Ion Implantation

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Single-Cell Metabolic Data Correction and Application Based on ToF-SIMS

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Minzu University of China

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) delivers a maximum spatial resolution on the submicron order of magnitude, and it is a vital technical platform for single-cell metabolic analysis[1]. During the acquisition and analytical procedures of single-cell metabolic data, ToF-SIMS measurements are susceptible to non-biological confounding factors, including sampling location differences, experimental batch fluctuations and instrumental status variations. These factors introduce prominent systematic errors, thereby impairing data stability and comparability, as well as the reliability of subsequent biological interpretation.Focusing on large-scale single-cell metabolic datasets acquired by ToF-SIMS, this study systematically compared the performance of multiple data correction methods, including raw processing, TIC normalization, Si signal normalization, Norm-SVR and SERRF. Based on the optimized correction outcomes, in-depth analysis of metabolic heterogeneity in A549 single cells was conducted, revealing the continuous and intrinsic metabolic heterogeneity within A549 single-cell populations.This research provides a methodological foundation and practical reference for improving the data quality of ToF-SIMS-based single-cell metabolomics, enhancing the comparability of results across independent experiments, and further elucidating the differential metabolic states within tumor cell populations（Figure 1）.

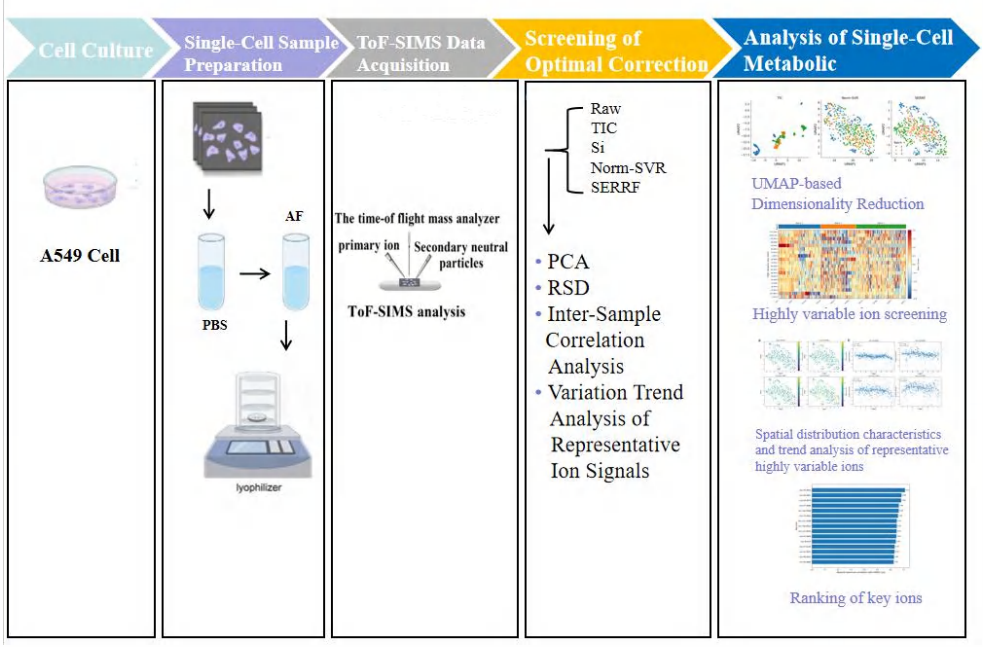


Figure 1 Experimental workflow

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Correlative imaging of secondary ion mass spectrometry and scanning electron microscopy at cryogenic temperature

Jiaqi Luo[1], Andrew Stallwood[1], Matija Lagator[1] Chelsea Norman[1], Ravi Teja Ravi[1], Thomas Glen[1], Jianguo Zhang[1], Maud Dumoux[1], Gwyndaf Evans[1], Felicia Green[1],

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Increasingly it is understood that using bulk analysis to understand disease progression within the human body misses the subtleties - be it infiltration of subsets of immune cells, hypoxic niches and metabolism microenvironments, or metastatic progression and the mechanical microenvironment. Therefore, direct tissue or cell imaging techniques are crucial in bioscience, but samples can be precious, hard to obtain or hard to prepare for analysis. A multiscale and correlative approach to extract the most information to understand a system can be extremely valuable.

In this work, we explored the possibility to bridge two imaging techniques at cryogenic temperatures: secondary ion mass spectrometry (SIMS) and scanning electron microscopy (SEM), which were performed on the very same positions of the same samples, aiming to extract correlative information. Preliminary experiments include investigation of: the effectiveness of the $(H_2O)_n^+$ Gas Cluster Ion Beam (GCIB) on cryogenic samples, and the effect of electron beam scanning on the chemistry observed in SIMS. Meanwhile, we have designed and manufactured a transfer system, capable of carrying a cryogenic sample stub suitable for transfer into, and analysis, by both instruments (Ionoptika J105 SIMS and ThermoFisher Hydra SEM). This enables successful transfer of ice-free samples between the instrumentation.

We aim to demonstrate the possibility of chemical and spatial imaging through the combination of SIMS and SEM at cryogenic temperature, which would enable mapping and navigation through complex biological samples while maintain integrity in their near-native state. This is illustrated through initial correlative SEM-SIMS images of chlamydia infected HeLa cells.

Evaluation of depth resolution and reconstruction of layered structure upon SIMS depth profiling by the three analytical models

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The three analytical models that are widely used for quantitative SIMS depth profiling, i.e. the atomic mixing-roughness-information depth (MRI) model [1], the up-and-down slope (UDS) model [2] and the roughness-cascade mixing-recoil (RMR) model [3], are systematically discussed. Firstly, the profile characteristics of the three models are analyzed according to definition, formula derivation and simulation analysis. Then, these models are compared in details with the partial depth resolution functions, the depth resolution function, the analytical expressions of analyzed thick film layer and the fitting of experimental data. Finally, the shortcomings of the UDS model are explained, and the incorrect description of the RMR model are corrected. Finally, as examples, some measured SIMS data are quantitatively analyzed for the evaluation of depth resolution and the reconstruction of layered structure in order to demonstrate the reliability and superiority of the MRI model.

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25th International Conference on Secondary Ion Mass Spectrometry

大连理工大学 DALIAN UNIVERSITY OF TECHNOLOGY

ToF-SIMS Reveals Biochemical Differentiation Across Corneal Layers in Mouse

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Background

The mouse cornea is composed of three anatomically distinct layers—the epithelium, endothelium, and stroma—each exhibiting markedly different physiological functions in maintaining transparency, providing barrier integrity, regulating immune privilege, and facilitating metabolic activity. Despite well-documented histological and functional differences among these layers, a systematic, high-resolution characterization of their in situ molecular-level chemical heterogeneity remains largely lacking. Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) offers label-free, sub-micrometer spatial resolution for chemical imaging combined with high-sensitivity spectral acquisition, making it a powerful tool to resolve region-specific molecular fingerprints in stratified tissues such as the cornea. In this study, we employed ToF-SIMS to systematically profile the chemical composition of the mouse corneal epithelium, stroma, and endothelium, aiming to identify layer-specific characteristic ion peaks, delineate distinct chemical fingerprints across the three layers, and provide a novel molecular-scale foundation for corneal physiology, pathology, and biomarker discovery.

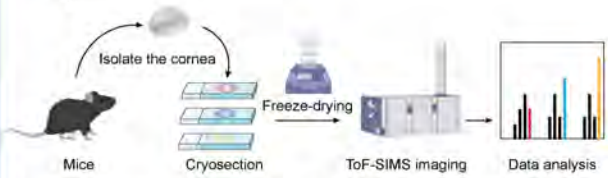


Figure.1 Experimental workflow. Main steps include: corneal dissection, cryosectioning of the three layers, ToF-SIMS data acquisition, spectral preprocessing, feature filtering, multivariate statistical analysis, and chemical imaging.

Methond

Corneal tissues from left eyes of male C57BL/6 mice were cryosectioned at 10 µm. ToF-SIMS analysis was performed using a Bi^{3++} cluster ion source at 60 keV over a 300 × 300 µm² scan area. Raw spectra were reconstructed and normalized to total ion intensity using Surface Lab 7.4. Peaks with intensity > 1×10⁻⁴TIC were selected, yielding ~500 peaks in positive mode and ~600 in negative mode. Features were then filtered by intra-group CV (threshold 0.35) and one-way ANOVA ($p < 0.05$), resulting in ~200 high-quality features. Principal component analysis (PCA) was then performed to resolve chemical differences among the three corneal layers.

Result

ToF-SIMS analysis revealed significant compositional differences among the mouse corneal epithelium, stroma, and endothelium. Principal component analysis (PCA) successfully separated the three layers into three distinct clusters, confirming their distinguishable overall chemical fingerprints. The loading plot identified more than seventy ions as major contributors to the separation, which were highly consistent with the heatmap screening results (m/z 184.07). Quantitative comparison of the normalized intensities of these characteristic ions showed that the intensity of the phosphocholine headgroup in the epithelium was more than 100-fold higher than that in the stroma ($p < 0.01$), while the endothelium exhibited a higher Cl signal (m/z 34.97). Chemical imaging further visualized that the m/z 184.07 signal was predominantly localized in the epithelial and endothelial layers, whereas the m/z 34.97 signal was uniformly distributed throughout the stroma.

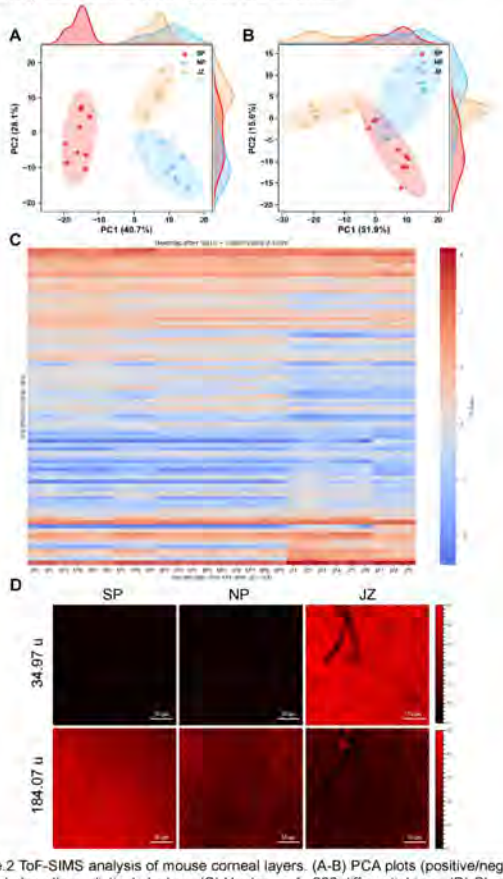


Figure.2 ToF-SIMS analysis of mouse corneal layers. (A-B) PCA plots (positive/negative modes) show three distinct clusters. (C) Heatmap of ~200 differential ions. (D) Chemical images: Cl⁻ (m/z 34.97) uniform in stroma; phosphocholine (m/z 184.07) enriched in epithelium/endothelium. Scale bar: 50 µm.

Conclusion

This study revealed significant and reproducible chemical fingerprints distinguishing the mouse corneal epithelium, stroma, and endothelium.

These characteristic ions may serve as layer-specific molecular signatures, and the approach can be extended to corneal disease models and tissue engineering.

Understanding SEI Formation at Polymer Electrolyte/Sodium Metal Interface: In-situ and post-mortem analysis via ToF- and Orbitrap-SIMS

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Solid polymer electrolytes (SPEs) such as poly(ethylene oxide) (PEO) are seen as promising candidates for solid-state sodium batteries. They ensure favorable interfacial contact with the electrodes while reducing overall device weight, allowing a high energy density. However, the high chemical reactivity of metallic sodium still hinders the use of organic components as electrolytes: solid electrolyte interphase (SEI) formation can translate in heavy consumption of active material and dendritic growth can potentially compromise long-term cell performance.

In this work, a PEO-based solid polymer electrolyte containing sodium bis(trifluoromethanesulfonyl)imide (NaTFSI) is investigated, to assess it´s reactivity toward metallic sodium, and to study the interphase formation and composition. Coulometric Titration Time Analysis[1] (CTTA) is employed to monitor SEI growth, directly linking it to side reactions between sodium and the polymer electrolyte. Post-mortem Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), coupled with Orbitrap-SIMS analysis characterizes the interphase formed on the current collector providing insights into its composition, structure and underlying growth mechanisms. An in-situ approach is further implemented to capture the dynamic nature of the interphase formation, using flood-gun plating directly on the pristine electrolyte surface within the SIMS instrument. This combined approach shows how the interphase is mostly composed by inorganic components, due to reactions of conducting salt with the plated alkali metal.

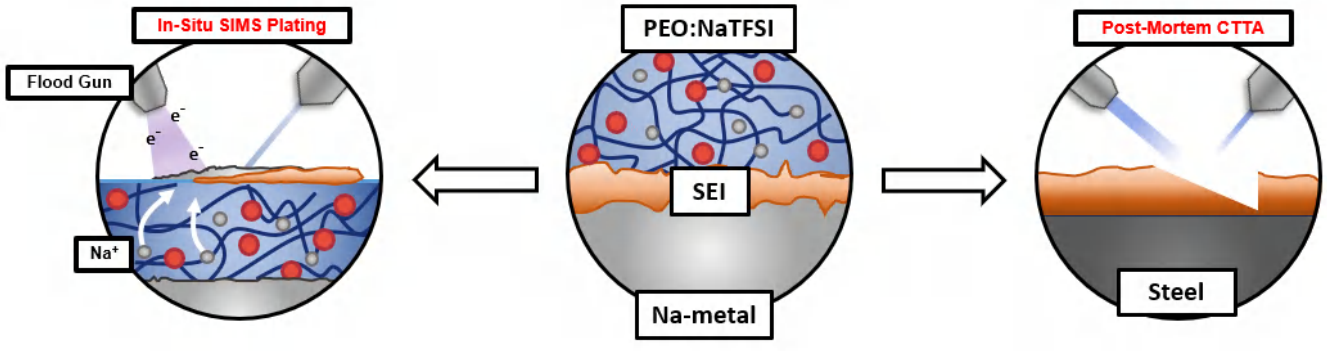


Fig. 1: Schematic illustration of the analysis

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Spatially Resolved SIMS Investigation of ALD-Derived Al_2O_3/TiO_2 Composite Coatings on Ni-Rich NCA Cathodes for Long-Cycle-Life Lithium-Ion Batteries

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Ni-rich layered oxide cathodes such as $Li[Ni_{0.8}Co_{0.15}Al_{0.05}]O_2$ are attractive for high-energy lithium-ion batteries, but their long-term cycling stability is limited by surface reconstruction, electrolyte decomposition, transition-metal dissolution, and cathode–electrolyte interphase evolution [1]. Here, we use a correlative SIMS approach to investigate how an atomic-layer-deposited Al_2O_3/TiO_2 composite coating modifies the surface and near-surface chemistry of Ni-rich NCA cathode particles. Complementary structural and electrochemical characterization showed that an optimized 2 nm-thick coating preserved the layered NCA structure and markedly improved capacity retention after 200 cycles at 1 C, thereby indicating the importance of nanoscale surface chemistry in stabilizing the cathode interface [2].

ToF-SIMS depth profiling was performed on pristine and coated NCA electrodes before and after cycling. Secondary-ion fragments related to electrolyte-derived and metal-fluoride interphase species, including POF_2^-, C_2F^-, $AlOF_2^-$, and NiF_3^-, were monitored as a function of sputtering time. Compared with the pristine electrode, the ALD-coated electrode showed lower POF_2^-, C_2F^-, and NiF_3^- signal intensities after cycling, suggesting the suppression of $LiPF_6$-derived decomposition, fluorinated organic species formation, and Ni-F-related surface degradation. The relatively enhanced $AlOF_2^-$ signal from the coated sample is consistent with the involvement of the Al-containing oxide layer in fluoride/oxyfluoride-rich interphase chemistry, rather than a purely inert physical barrier.

Nano-SIMS imaging was further used to visualize the lateral distributions of $^7Li^{16}O^-$, $^{16}O^-$, $^{27}Al^{16}O^-$, and $^{48}Ti^{16}O^-$ secondary ions across individual secondary NCA particles. The Al- and Ti-containing oxide fragments were detected over the particle surface, supporting the presence of an ALD-derived protective layer, while the Li^- and O^- related signals provided spatial information on particle-scale chemical variations in the cathode surface and near-surface region. These results demonstrate that ToF-SIMS and Nano-SIMS provide complementary depth-resolved and spatially resolved information on cathode–electrolyte interphase formation [3].

This work shows that the ALD-derived Al_2O_3/TiO_2 coating regulates interfacial degradation pathways by suppressing electrolyte-derived phosphate/fluorocarbon fragments and Ni–F-rich surface species while promoting Al/Ti oxide-derived passivation chemistry. The results highlight the capability of correlative SIMS analysis to link nanoscale interfacial chemistry with electrochemical durability in high-Ni cathode materials.

Acknowledgement
This research was supported by the Korea Industrial Technology Association (KOITA) grant funded by the Korea government (Ministry of Science and ICT) (2710093406).

Keywords: ToF-SIMS depth profiling, Nano-SIMS imaging, Ni-rich NCA cathode, ALD coating, Al_2O_3/TiO_2, cathode–electrolyte interphase

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Urban mining assisted by ToF-SIMS

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Modern building materials gain their advanced properties by the use of additives and additive combinations. While gypsum in principle can be fully recycled, the additive cocktail may pose challenges for the recycled product or the process itself. Especially the presence of unknown additives is critical, restricting urban mining to materials of known origin. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) has the potential to determine the additive composition unambiguously, thus allowing educated selection of adapted additive cocktails to efficiently recycle previously unusable material from urban mining or landfill sources. ToF-SIMS analysis may be a powerful addition in the material sorting process, enabling targeted recycling strategies also for gypsum from unknown origin. An optimized configuration for analysis of building materials was developed, a data base of common additives in gypsum industries was created and the potential of the technique as support for urban mining was evaluated.

NanoSIMS imaging – A powerful tool to reveal nanostructures and quantify trace elements in life and Earth sciences

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The nanoscale secondary ion mass spectrometry (NanoSIMS) is a unique secondary ion nanoprobe capable of measuring elemental, isotopic, inorganic, organic, and biomolecular distributions with high sensitivity (down to ppm levels), as well as providing 2D and 3D imaging with nanometer spatial resolution (~50 nm laterally and 10 nm axially). NanoSIMS has been increasingly applied in various research fields, especially in life, Earth, environmental, and materials sciences, to visualize nanoscale structures and quantify trace elements. Its power is further enhanced when combined with other imaging techniques, such as fluorescence microscopy, electron microscopy, atomic force microscopy, and atom probe tomography, to obtain comprehensive and complementary information from the same sample.

Here, we present a showcase of NanoSIMS applications demonstrating the potential of this technology to characterize protein turnover in human neural progenitor cells at the organelle level [1], track the accumulation and quantify antisense oligonucleotide drugs in single human hepatocyte cells [1], and measure hydrogen concentrations in the most abundant mineral on Earth [3,4]. NanoSIMS imaging, with its capability to correlate with other imaging techniques, offers a new window for exploring chemical ultrastructures, revealing complex sample properties as well as the relationships between sample structure and function.

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Nanoscale Chemical Imaging with a Novel Liquid Ionic Compound Ion Source (LICIS) Coupled to O-TOF-SIMS

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Recent advancements in nanoscale material characterization – covering battery technologies, microelectronics, and metallurgy – demand highly resolved analytical techniques capable of correlative and multi-modal analysis. While Secondary Ion Mass Spectrometry (SIMS) remains the gold standard for chemical imaging at the nanoscale, its performance is critically limited by the primary ion source. Traditional ion sources such as Liquid Metal Ion Sources (LMIS), Surface Ionization Sources, Plasma Sources or Gas Cluster Ion Beams offer distinct trade-offs between spatial resolution, secondary ionization yield, and ion species diversity, often compromising one for the other.

To address these challenges, we introduce a novel Liquid Ionic Compound Ion Source (LICIS), designed to generate stable, high-brightness and highly reactive ion beams (e.g., Cs^+, NO_3^-) from ionic liquids of molten salts (Figure 1). Coupled with Orthogonal Time-of-Flight SIMS (O-TOF-SIMS), this new system leverages the pulsed secondary ion extraction of O-TOF-SIMS achieving sub-30 nm spatial resolution and a mass resolution exceeding 4,500 (FWHM on ^{28}Si) [1]. Integrated into the UHV NanoSpace platform (Tescan France), this setup enables in-situ correlation of SIMS with SEM, STEM, EDX and EBSD for comprehensive 3D chemical and structural analysis [1,2]. The capabilities of LICIS coupled with O-TOF-SIMS have been demonstrated through challenging applications in microelectronics.

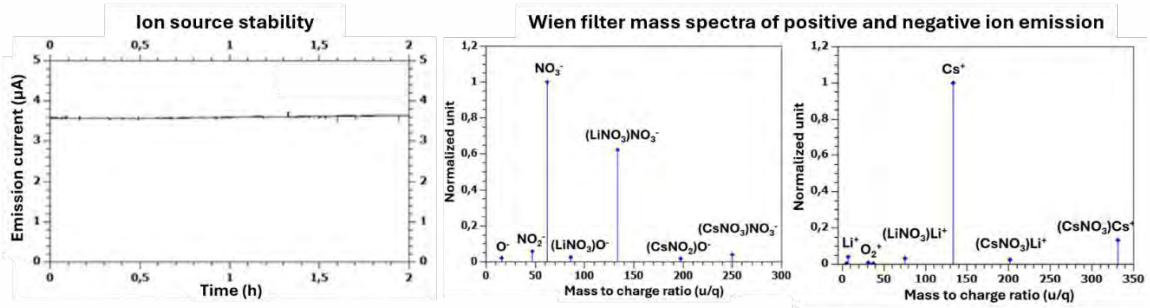


Figure 1: Ion source emission stability over two hours and wien filter mass spectra of positive and negative ion emission.

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Three-Dimensional SIMS and Machine-Learning-Assisted Spectral Informatics for Assessing Surface Chemistry Evolution in Reused GH3536 Superalloy Powder

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Powder reuse in laser powder bed fusion can alter the near-surface chemistry of Ni-based superalloy powders, yet the changes are often confined to thin, chemically heterogeneous layers. Here we combine three-dimensional TESCAN Nanospace-SIMS analysis with an automated ToF-SIMS interpretation workflow to evaluate elemental consistency between virgin and once-reused GH3536 alloy powders. Positive- and negative-ion datasets were acquired over a 30 μm × 30 μm × ~10 μm volume with 400 × 400 × 2000 voxels; to reduce edge-sputtering artefacts, the central 320 × 320 × 2000 voxel region was used for quantitative comparison. Elemental signals were normalized to the total ion signal. In parallel, exported HDF5 spectra were processed by a local machine-learning-assisted pipeline incorporating mass-axis calibration, peak integration, isotope-pattern backfilling, full-element screening, and tiered element assessment.

Depth profiling reveals that powder reuse primarily modifies the surface and near-surface chemistry. Oxygen enrichment forms a continuous oxide layer whose apparent thickness increases from ~300 sputter layers in the virgin powder to ~400 layers after reuse. Boron, carbon and hydrogen show stronger near-surface enrichment in the reused powder, while fluorine is concentrated at the outermost surface. Sulfur exhibits localized enrichment, indicating increased chemical heterogeneity. In contrast, the principal alloying elements Ni, Cr and Fe remain comparatively uniform with depth and show no pronounced batch-dependent segregation. Three-dimensional ion maps further demonstrate enhanced clustering and spatial inhomogeneity of light-element and oxide-related signals after reuse. The automated spectral assessment independently confirms robust Ni/Cr/Fe/Mo alloy signatures in positive-ion spectra and flags trace or overlapping species for review rather than direct assignment.

Overall, the results indicate that one reuse cycle preserves the bulk elemental consistency of GH3536 powder but promotes surface oxidation, light-element segregation and microscale chemical heterogeneity, highlighting the value of 3D SIMS combined with auditable spectral informatics for powder lifecycle qualification.

Key words： GH3536 superalloy powder; powder reuse; 3D SIMS; ToF-SIMS; surface oxidation; machine learning; additive manufacturing

In-situ Liquid ToF-SIMS Analysis of Water Cluster

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The dynamic contraction of hydrogen bonds within various water clusters underlies water's unique physicochemical properties. Arrangements of water clusters with different size and structure is of vital significance to phase change, solvation process, biomacromolecular conformation, and etc. However, most of mass spectrometry relying on high vacuum degree restricts liquid experiments. In in-situ liquid ToF-SIMS, a liquid-filled closed chamber is affixed to the sample holder. A micro analysis window is milled by bismuth source on the chamber surface. The high surface tension of water at the micropore confines liquid within the chamber, allowing in-situ dynamic detection of water clusters.

In our work, we built a microfluidic chamber for in-situ chemical reaction. A wide range size clusters of pure and heavy water was observed, demonstrating robustness and repeatability of our method. Subsequently, we analyzed how halogenated anions and pH influence water clusters and found that hydrogen-bond network can be disrupted by larger halide anions and strengthened by free protons, respectively. Besides, our work shows the significance of nuclear quantum effects, providing important insights in water research.

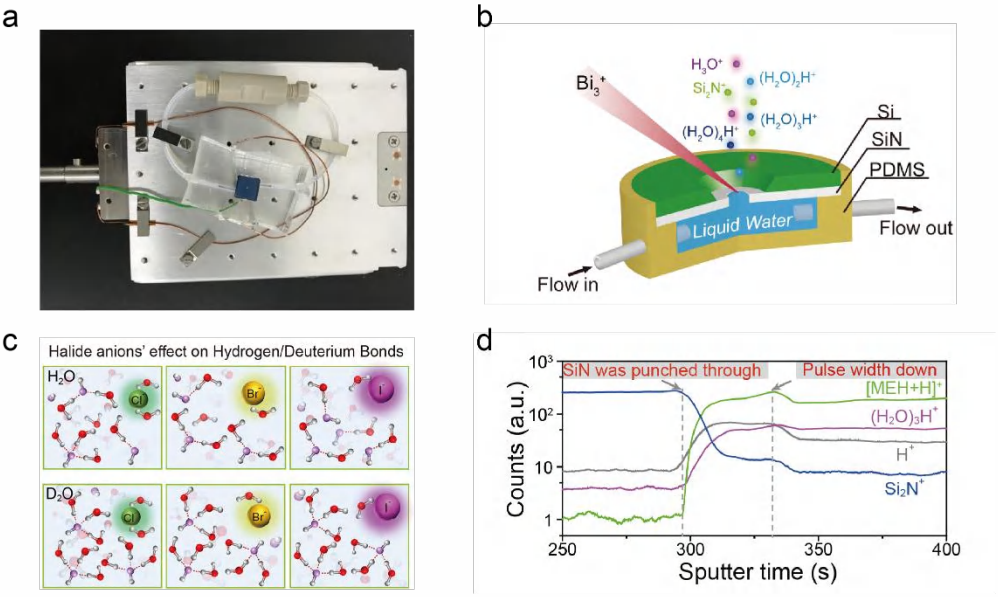


Figure 1. Schematic of in-situ liquid ToF-SIMS and characterized water clusters.

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Machine Learning Approaches for ToF-SIMS Data Interpretation: Supervised and Unsupervised Methods

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Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) enables the simultaneous acquisition of chemical composition (m/z) and its spatial distribution within a sample, making it an indispensable tool for materials characterization. However, a single ToF-SIMS measurement typically yields a hyperspectral dataset comprising hundreds of mass peaks across tens of thousands of pixels, and analyzing such high-dimensional data across a large number of samples is both time-consuming and difficult to interpret comprehensively. Conventional analysis often requires selecting a limited number of representative peaks or integrating spectra over regions of interest, which risks discarding chemically or spatially relevant information. Multivariate analysis and machine learning techniques address this limitation by allowing the full mass range and pixel-level spatial information to be analyzed directly and simultaneously. In this study, we report two complementary applications of these techniques: an unsupervised approach for the exploratory, comprehensive interpretation of ToF-SIMS hyperspectral data, and a supervised approach for quantitative depth-profiling.

We first present case studies in which multivariate analysis techniques such as Principal Component Analysis (PCA) and Multivariate Curve Resolution (MCR), along with machine learning methods such as Sparse Autoencoders (SAE), were applied to model systems representative of materials under development, without compressing either the mass or spatial dimensions of the data. The effectiveness of these approaches for interpreting ToF-SIMS hyperspectral images has been demonstrated in recent studies[1], and here we extend its application to industrially relevant model systems.

As a second example, we address the challenge of quantification in ToF-SIMS, which arises because secondary ion yields are strongly matrix-dependent, making direct quantification from spectral intensities alone difficult. To overcome this limitation, we demonstrate a supervised machine learning approach that combines ToF-SIMS spectral data with quantitative results from complementary techniques such as X-ray Photoelectron Spectroscopy (XPS) and X-ray Absorption Fine Structure (XAFS). Leveraging the high depth resolution of ToF-SIMS, this approach was used to predict the mixing ratio of a bilayer stacked film at each sputtered depth, demonstrating the feasibility of machine learning-assisted ToF-SIMS analysis for quantitative, depth-resolved characterization of layered materials.

The authors would like to thank Prof. Satoka Aoyagi (Seikei Univ.) for valuable discussions and technical assistance with the ToF-SIMS data analysis.

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TOF-SIMS laboratory at Guangdong Technion

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Alongside the ongoing trend of globalization, academia must meet the international demand for more innovative and sophisticated education to prepare new generation of engineers and scientists to learn from the past and to build future expertise particularly in the area of surface analysis. The research of the elusive zone where surface and subsurface of the solids interacts directly or just "feel" the power of the external environment is the focal point for development of a wide range of modern technologies, including semiconductors, nuclear or aviation industry.

In this regard, we introduce a Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) laboratory, established at Guangdong Technion-Israel Institute of Technology (GTIIT), which is a Sino-foreign cooperative university jointly funded by the Technion (Israel) and Shantou University (STU), located in Shantou City, Guangdong Province. From the outset, it was essential to gather state-of-the-art surface analysis tools under one roof to support both research and the educational development of our students. To this end, a multidisciplinary research center was built, offering internal and external users access to a modern, up-to-date research facility. This includes ToF-SIMS facility and complementary laboratories, such as XPS, AFM, XRD.

The poster highlights the capability of ToF-SIMS laboratory at GTIIT through selected examples of recent work, covering the following topics:

1) Isotopic labelling with ^{18}O to study flow mechanisms during the anodization of light metals and alloy surfaces [1]

2) Depth profiling of solid-electrolyte interphase components in high-voltage lithium batteries to evaluate modified electrolyte performance [2].

3) Elemental distribution analysis of anodic titanium oxide nanotubes decorated with tin oxide via atomic layer deposition, for potential application in seawater splitting to generate hydrogen [3]

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Interfacial Adsorption in Semiconductor Devices Unveiled by ToF-SIMS and XPS

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Controllable adsorption of molecular surface modifiers is essential to device stability and process reliability in advanced electronics. As packaging adopts complex, multi-component metal/alloy substrates, characterizing interface adsorption grows critical yet analytically demanding. Conventional techniques such as XPS lack sensitivity for trace adsorption, leaving the substrate–modifier interplay poorly resolved. Here, we combine ToF-SIMS, PCA, and XPS to quantify polysiloxane modifier adsorption on bare/passivated Cu, Ag with/without a protective layer, and pre-plated frames (PPF). We find that protective layers dominate interfacial adsorption: passivated Cu adsorbs markedly more Si than bare Cu, where the native oxide suppresses uptake. PCA of ToF-SIMS data distinguishes substrate-specific adsorption regimes and identifies the principal chemical signatures underlying substrate differentiation. ToF-SIMS demonstrates superior sensitivity to XPS for trace-level quantification and confirms PPF adsorption, providing a substrate-resolved route for interface engineering in advanced packaging.

Key words: ToF-SIMS; XPS, PCA, Interfacial adsorption

Isotopic labelling study of Oxygen and Hydrogen in surface analysis

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Isotopic labelling with stable isotopes, such as oxygen-18 (^{18}O) or deuterium (D) combined with Time of Flight Secondary Ion Mass Spectrometry techniques (ToF-SIMS) and particle accelerator-based techniques, represent powerful tools for identifying, tracking and quantifying ion migration under diverse technological conditions. Despite the well-established use of isotopic tracing in silicon technology since the early 1970s, its application in applied electrochemistry or surface science to explore phenomena at the nanoscale remains relatively understated and unexplored by non-physicists.

This talk considers two set of methods: (i) ToF-SIMS and (ii) ion beam analysis (IBA), which utilizes specific nuclear reactions performed at tandem or Van de Graaff accelerators. Both techniques are well-established in physics and chemistry thanks to significant improvements in vacuum technology and detector systems and both belong to a relatively narrow range of techniques sensitive to isotope detection.

In this context, examples of quantitative and qualitative analyses of ^{18}O tracer in thin aluminum oxide and titanium films will be presented through a comparison of Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS), Nuclear Reaction Analysis (NRA), Narrow Resonance Depth Profiling (NRDP) [1], and Elastic Recoil Detection Analysis (ERDA) applied to deuterium (D) tracing for optimizing atomic layer deposition (ALD) formation of titanium oxides [2].

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Genetically Encoded Fluorine Deposition Enables Colorized Electron Microscopy

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Abstract Content:

Nanoscale ultrastructure and molecular distribution determine cell functioning, especially the delicate information processing of neurons. While electron microscopy visualizes subcellular ultrastructure peerlessly, localizing biological molecules at nanoscale requires compatible molecular markers. The popular fluorescent protein markers suffer from the harsh fixatives necessary for ultrastructure preservation while most electron diffracting markers requires membrane penetration for successful delivery. Here, we introduce genetically encoded fluorine deposition as an electron microscopy-compatible marker to overcome the limitations. By utilizing a peroxidase APEX2 and a stable, commercially available fluorine-containing substrate, bisphenol AF (BPAF), we succeeded in targeted deposition of fluorine. Fluorine deposition provided a clear contrast based on its rarity in living systems, survived heavy metal ion staining and epon embedding by its chemical stability, and avoided obscuring the endogenous structural contrast. Distribution of fluorine and thus the target was mapped with nanoscale secondary ion mass spectrometry (nanoSIMS). NanoSIMS maps molecules carrying unique element or isotope at sub-optical resolution on the same ultrathin section as scanning electron microscopy. As a demonstration, organelles including mitochondria, and the α-tubulin molecule, were highlighted in human embryonic kidney cells (HEK 293T) by combined mapping with nanoSIMS and scanning electron microscopy. This specific and easy-to-use fluorine marker opens the possibility of multi-colored nanoscale imaging with multiple elements and isotopes.

Key words: fluorine, APEX2, electron microscopy, nanoSIMS, molecular marker.

DSIMS characterization of P doping in a trench SiC sample

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Abstract

Dynamic Secondary Ion Mass Spectrometry (DSIMS) is suitable to detect dopants in the samples with smooth and flat surface. If the sample surface is non-planar, it will affect the data accuracy. This paper presented a experiment to detect the dopants in a trench sample using DSIMS. The trench was filled with SiO_2 before DSIMS test. The obtained results showed that the filled sample had more accurate profile compared to the one without trench filling.

Introduction

Dynamic Secondary Ion Mass Spectrometry (DSIMS) is a surface tool. It applies a primary ion beam to bombard the sample surface and collect the information of the secondary ions from the bombarded surface. The primary beam continually erodes the samples and obtains the ion profiles with depth, so it is called “dynamic” SIMS [1]. It is suitable for solid samples with flat and smooth surface. However, for traditional non-planar samples, the depth profiles DSIMS obtains may not be accurate. Because erosion rates of trench and mesa are different, the secondary ions emitted from the sample are not from the same depth.

In this work, a trench SiC was doped with phosphorus (P), where the P was in the mesa walls and trench bottom. DSIMS was applied to characterize the P depth profile in the sample. In the first experiment, DSIMS directly tested on the original sample. However, due to the P ions emission from different depth, the data looks wired. In the second experiment, the sample was improved by filling trench with SiO_2 via Chemical Vapor Deposition (CVD) experiment. The trench sample became planar sample. DSIMS was performed on this improved sample. The data was further corrected due to the trench geometry.

Experimental

In this study, a trench SiC was doped with phosphorus (P), where the P was in the mesa walls and trench bottom. The schematic structure of the sample is shown in Fig. 1. DSIMS was applied to characterize the P depth profile in this SiC trench sample. In the first experiment, DSIMS directly tested on the original sample. In the second experiment, the trenches were filled with SiO_2 by CVD experiment. The ideal materials to fill the trenches is SiC, but due to our source constraint, filling SiC was not available. Considering DSIMS sputter rates of SiC and SiO_2 are similar, so we tried to fill the trenches with SiO_2. Fig. 2 shows the process of filling the trenches with SiO_2. Cameca IMS 7f DSIMS was used in this work.

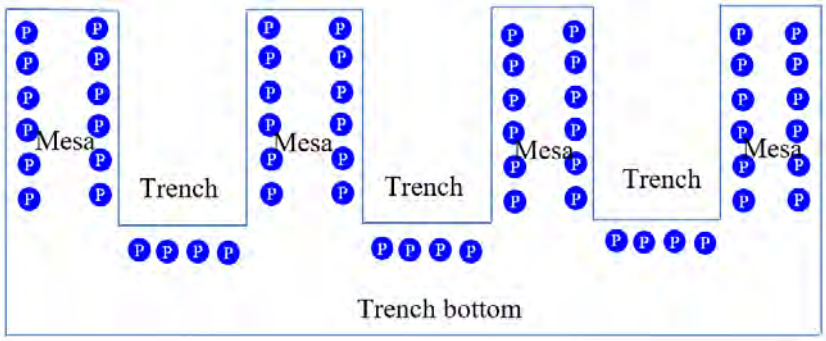


Figure 1. Schematic structure of the SiC trench sample. P dopants are in the mesa walls and trench bottoms.

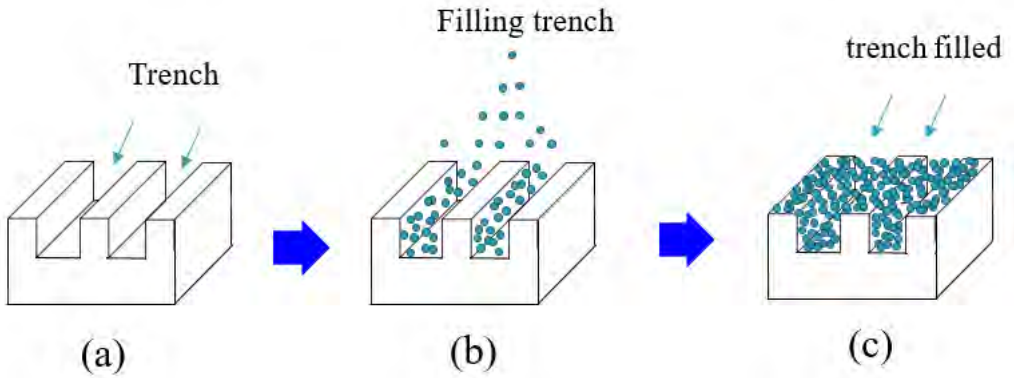


Figure 2. Schematic showing the trenches filled with SiO_2.

Results and discussion

Fig. 3 shows the DSIMS depth profile in the original sample. The green lines is the Si ion intensity and the red line is the P concentration with depth. It can be seen that the red line gradually increased when it is close to the trench bottom. It is because when the DSISM primary beam sputtered close to the trench bottom, it eroded the trench bottom and mesa together. The secondary ions came from both trench bottom and mesa. Therefore, the P signal increased at the end of the mesa. This data could not present the accurate P concentration depth profile.

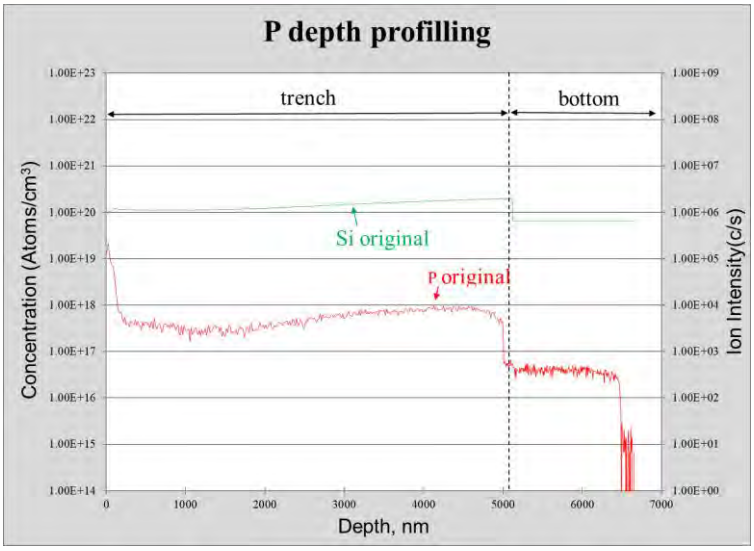


Figure 3. DSIMS depth profile in the original trench sample.

DSIMS data on the second experiment was presented in Fig. 4. In the second experiment, the trenches were filled with SiO_2. The as-measured DSIMS data covered an area of 33x33um square, in which many trenches and mesas are inside. So it is needed to do a correction to recalculate the dopant concentration.

The dopant concentration was corrected by below formula (1) [2]:

C= C (original) * [(M+T)/M] (1)

Where C is the corrected dopant concentration;

C (original) is the original collected dopant concentration;

M is the area of mesas within the sputter area;

T is the area of trenches within the sputter area;

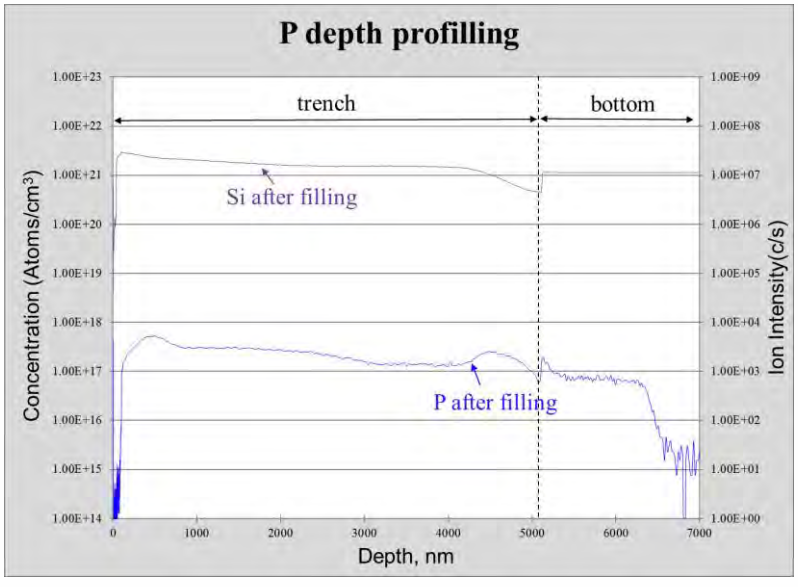


Figure 4. DSIMS depth profile in the SiO_2-filled sample.

The comparison of the depth profile between the original sample and trench-filled sample was presented in Fig. 5. It can be seen that P in the sample after filling trench did not show increase at the bottom of the mesa. Because the trenches were filled, the difference of the sputter rate between the mesas and trenches was much smaller than that of the original trench sample. In addition, the P signal at the bottom of the original sample is lower than the filled sample. It is also due to the different sputter rate between the trenches and mesas. The depth profile of the sample after filling-trench looks more logical and closer to expectation.

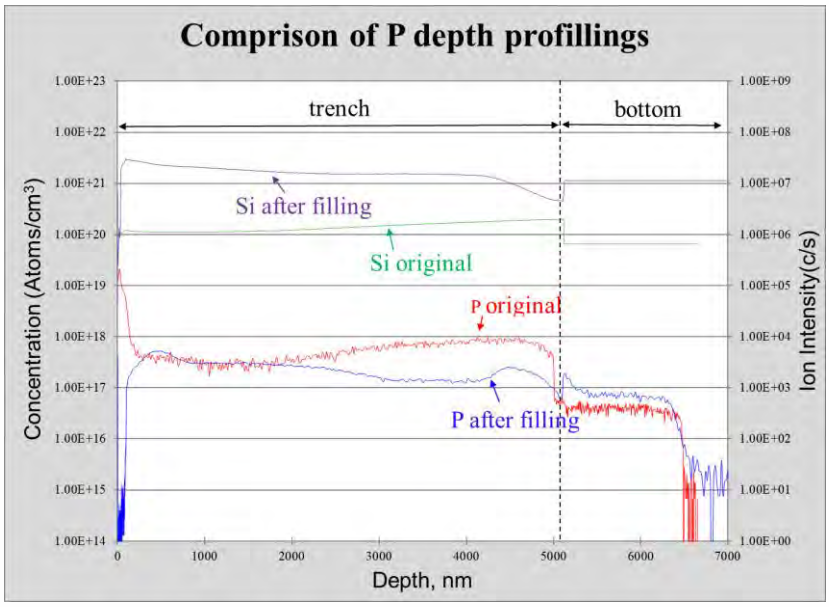


Figure 5. Comprison of DSIMS depth profiles in the original and SiO_2-filled samples.

Conclusions

In this work, DSIMS was used to characterize P concentration depth profile in a trench SiC sample. The direct test on the trench sample was not accurate, due to the different sputter rate of the trench and mesa. The sample was improved by filling the trench with SiO_2 with our available source. DSIMS was performed on the improved sample. Further correction was done on the data due to trench geometry. Above two data was compared and the latter one showed more logical and closer to expectation.

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Cryo ToF-SIMS to Study Sodium Transport and Storage in Hard Carbon Anodes

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Among anode materials for sodium-ion batteries (SIBs), hard carbon has emerged as the most promising candidate owing to its relatively high reversible capacity, moderate operating potential, and compatibility with standard electrolyte systems. Despite considerable progress, the underlying sodium transport kinetics and storage mechanisms remain insufficiently understood, hampering the rational design of high-rate electrodes. Conventional electrochemical techniques such as galvanostatic intermittent titration (GITT) yield macroscopically averaged kinetic parameters but cannot resolve the spatial distribution of sodium within the carbon microstructure. To overcome this limitation, we employ thin-film model electrodes and investigate sodium transport and storage by ToF-SIMS in a controlled diffusion experiment.

Resol-resin-derived hard carbon thin films, deposited under well-defined conditions, replicate the essential structural features of electrode-grade hard carbon while eliminating the geometric complexity inherent to porous composite electrodes. Sodium is deposited on these films via physical vapour deposition, establishing well-defined initial concentration profiles. Subsequent ToF-SIMS depth profiling tracks the temporal evolution of the sodium distribution at varying temperatures, providing spatially resolved diffusion data inaccessible by electrochemical methods alone. Given the exceptionally fast sodium transport and high reactivity, all diffusion experiments are performed in situ within the SIMS instrument under cryogenic conditions.

A critical prerequisite is verifying that the thin-film material faithfully represents the microstructure of composite electrodes. Transmission electron microscopy (TEM) compares local structures at the nanoscale, with particular focus on pore size distributions in both thin films and practical electrode materials. This structural validation establishes the link between the model system and real-world electrode conditions, lending credibility to the calculated diffusion coefficients. To derive quantitative diffusion coefficients from the SIMS depth profiles, a finite element diffusion model extracts concentration-dependent values, yielding improved consistency with GITT measurements and accurately reproducing experimental depth profiles.

In summary, integrating thin-film model electrodes, temperature-dependent ToF-SIMS depth profiling, TEM structural characterisation, and grain-based finite element modelling affords unprecedented spatial and temporal resolution of sodium diffusion mechanisms in hard carbon, providing essential insights for rational anode design in next-generation SIBs.

Identifying key materials in ancient hearth stones from the late Pleistocene era using SIMS and machine learning

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Analysing ancient artefacts [1,2] requires a high level of sensitivity and the ability to identify unknown materials. Moreover, the artefacts also contain contaminants that have been adsorbed onto them over time and during the burial, excavation, and curation. Secondary ion mass spectrometry (SIMS), such as time-of-flight SIMS (ToF-SIMS), that can analyse solid samples directly and, with its high sensitivity and depth-direction analysis capabilities, is one of the most powerful techniques for identifying small amounts of materials remaining in ancient artefacts separated from the contaminants. However, ToF-SIMS using Bi cluster ion beams, the most common primary ion beam, produced mainly low-mass peaks below 100 Da, which were insufficient for identifying the molecules in the sample. Therefore, this study also used SIMS with gas cluster ion beams, such as Ar cluster and water cluster ion beams, to identify the molecules. The samples in this study were ancient hearth stone pieces of the late Paleolithic (ca. 15,000 BP), which were discovered in Hokkaido, Japan. These stones are assumed to have been used for cooking in the Palaeolithic period, due to the red and black surface colours and the contexts in which they were excavated, as well as the fact that lipids were recovered from them. The samples were measured using J105 Cluster SIMS (Ionoptika Ltd., Eastleigh, UK) and OrbiSIMS (ION-TOF GmbH, Münster, Germany) with Ar cluster ions. The SIMS depth profiles were analysed using unsupervised machine learning techniques, such as principal component analysis (PCA), multivariate curve resolution (MCR) and sparse autoencoder (SAE), to extract important features [3] related to the remaining materials and distinguish them from the contaminants. Supervised machine learning was also applied to the datasets to identify mass peaks specific to particular sample features [3]. As a result, the water cluster SIMS yielded characteristic mass peaks in the range of 200-700 Da. High mass peaks were also detected in the OrbiSIMS spectra and their origins were indicated. As a result, the existence of lipids and molecules derived from plants and marine products was indicated.

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Uncovering Organic Surface Chemistry: From Intentional Modification to Contamination Identification

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Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is uniquely suited to organic surface and interface analysis, combining extreme surface sensitivity, molecular specificity, and imaging capability. These attributes are particularly valuable in systems where even a monolayer or trace contamination redefines the surface chemistry of the substrate.

A prominent example is the use of self-assembled monolayers (SAMs) of amphiphilic molecules to engineer surface chemistry on silicon oxide substrates. SAMs organosilanes are widely used to engineer surface chemistry on silicon oxide surfaces including silicon wafers and glass substrates. Such monolayers are commonly applied to control wettability, enhance adhesion, or provide coupling layers between inorganic substrates and functional organic coatings. Because most organosilane SAMs are thinner than 2.5 nm, ToF-SIMS is uniquely suited to probe their chemistry. By examining inter-ion relationships among silicon-oxide cluster ions (e.g., $Si_2O_4H^-$, $Si_2O_5H^-$), ToF-SIMS can distinguish signals arising from the siloxane network of an organosilane monolayer from those of the underlying silicon-oxide substrate. This relation-based analytical approach, rather than relying on individual diagnostic ions when such ions are absent, significantly improves chemical selectivity for resolving structurally similar species.

In contrast to deliberately engineered surfaces, trace organic contamination can lead to serious performance issues in industrial processes. One of the major industrial applications of ToF-SIMS is the identification of extremely low levels of contaminants and micron-scale particles, where determining the origin of contamination is essential for effective elimination or mitigation. Based on a large body of industrial case studies, ToF-SIMS has demonstrated excellent sensitivity and chemical selectivity in identifying diverse classes of contaminant species that are responsible for coating failures.

Together, these examples demonstrate that ToF-SIMS is uniquely capable of detecting and characterizing trace-level quantities of organics that critically influence surface chemistry, whether as intentionally designed molecular layers used to modify and functionalize technologically important substrates, or as unintended contaminants that must be identified, traced to their origin, and effectively controlled.

Quantitative analysis using multilayer perceptron for organic electroluminecense material mixtures based on SIMS spectra treated with Hopfield neural network

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As secondary ion mass spectrometry (SIMS) is a highly sensitive surface analysis and a mass imaging method for two-dimentional and depth analysis of each substance, it has been applied to the evaluation of a variety of samples. However, SIMS spectra of organic samples are complex and matrix effects causie the intensity changes in particular secondary ions derived from a specific substance, regardless of its concentration, which makes quantitative analysis difficult. We have developed an artificial neural network (ANN) system for quantitative analysis of SIMS data in the Versailles Project on Advanced Materials and Standards (VAMAS) project TWA2 A31, using a supervised learning system based on a multilayer perceptron type of artificial neural network [1]. Although the ANN-based quantitative analysis was effective for two-component system of organic electroluminescent materials, interpreting important mass peaks to determine the ratio of target materials remained complicated. In this study, in order to extract more essential mass peaks information from the ANN analysis processes, the SIMS spectra used for training were treated with another ANN method, Hopfield Neural Network (HNN), which is a Recurrent Neural Network (RNN). HNN treated SIMS spectra were used as training data for the ANN quantitative analysis. As a result, the accuracy of the ANN quantitative analysis using HNN-treated SIMS spectra was high, and the essential mass peaks for each component in the samples were indicated by the weights of the ANN.

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Dynamic SIMS Characterization of Dopants in SiC for Advanced Power Electronics

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Silicon carbide (SiC) has emerged as a key wide-bandgap semiconductor for high-power, high-frequency, and high-temperature electronic applications. Continued progress in SiC device performance and reliability critically depends on precise control of both intentional dopants and unintentional impurities introduced during crystal growth and processing. Accurate characterization of low-level dopant concentrations and spatial uniformity is therefore essential.

In SiC, both n-type and p-type doping must be tightly controlled, with nitrogen and phosphorus commonly used as n-type dopants and aluminum as the primary p-type dopant. Reliable quantitative analysis of these dopants at low concentration levels and with microscale spatial resolution is therefore of key importance.

Dynamic SIMS remains a reference technique for elemental depth profiling and trace impurity analysis and is increasingly applied to wide-bandgap materials such as SiC, where high sensitivity, large dynamic range, and flexible depth profiling capabilities are required. Implemented on magnetic-sector instruments, dynamic SIMS enables reliable dopant and impurity profiling in SiC from near-surface regions down to several micrometers, as well as lateral assessment of compositional uniformity.

In this contribution, we present representative examples of SiC characterization using CAMECA magnetic-sector SIMS instruments. Analytical strategies and results are discussed for nitrogen, phosphorus, and aluminum dopant profiling, as well as selected impurity analyses and lateral uniformity measurements. These examples highlight how dynamic SIMS supports both materials development and process optimization for next-generation SiC-based electronic devices.

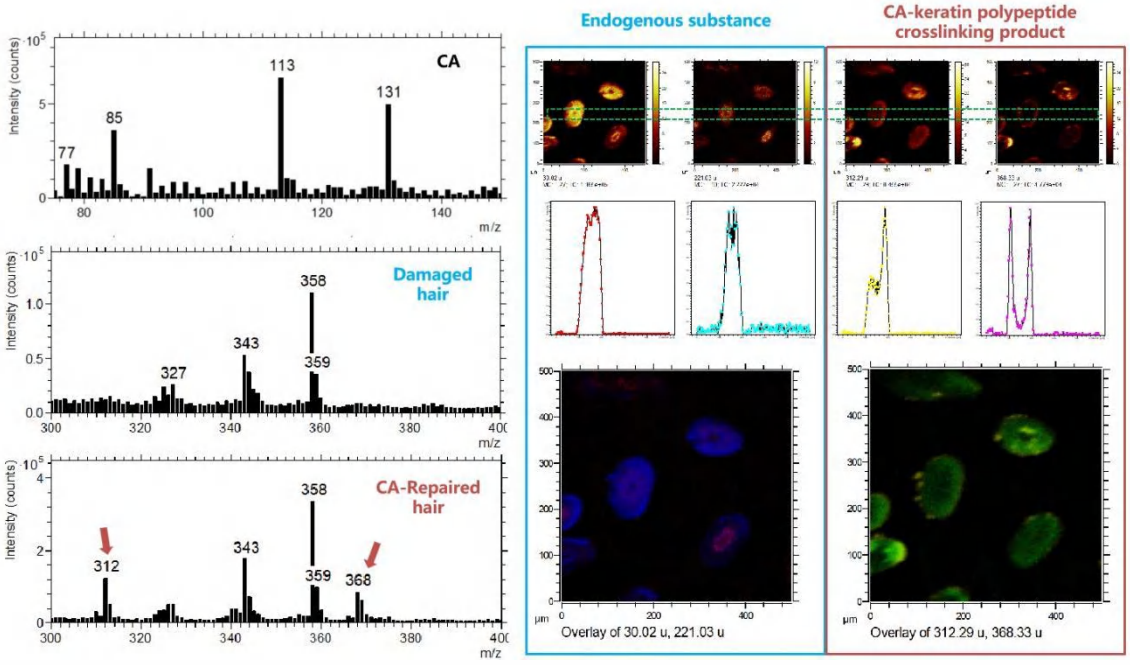
TOF-SIMS Characterization of the Layered Structure of Hair and Study of Repair Mechanisms

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In current hair care product development, problems such as a monolithic efficacy evaluation system and unclear mechanisms of action commonly exist. By taking advantage of the high mass resolution and high spatial resolution of TOF-SIMS, it is anticipated that the multi-layered structure of hair can be effectively identified and distinguished, thus offering technical support for further investigations into the penetration pathways and mechanisms of active ingredients within hair. Herein, the embedding and cryosectioning procedure for hair was initially optimized by substituting water for OCT, aiming to obtain secondary ion mass spectrometry samples free from OCT spectral interference and featuring a flat surface. Based on the new method sample preparation, TOF-SIMS mass spectrometry analysis and chemical imaging of hair cross-sections were then performed. The TOF-SIMS characteristic ions and their distribution of components including keratin and lipids within the hair matrix were clarified, and the layers in the cross-section, including the cuticle and cortex, were identified on the basis of chemical composition information. Meanwhile, as a small molecule active agent, the repair efficacy of citraconic acid(CA) on different hair layers is evaluated through comparison with damaged samples. It was found that the CA can undergo cross-linking reactions with keratin polypeptides. This study provides high-quality mass spectrometry data to support further exploration of the penetration pathways and mechanisms of active ingredients into hair.

Key words: SIMS; Hair; Layered structure; Characterization; Repair mechanism



Mapping SETBP1-Driven Molecular Disruption in Schinzel-Giedion Syndrome Using Correlative SIMS

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University of Gothenburg

Schinzel-Giedion syndrome (SGS) is a rare genetic disorder caused by de novo mutations in the degron of the SETBP1 protein, which prolong SETBP1 activity beyond its normal physiological role [1,2]. Since SETBP1 is involved in the regulation of gene expression, the mutation drive widespread molecular disruption across multiple spatial scales [3–5].
However, the relationship between tissue-level biochemical changes and single-cell dynamics remains poorly understood. Here, we apply a correlative secondary ion mass spectrometry (SIMS) approach to investigate these processes in a mouse model of SGS.
Time-of-flight SIMS (ToF-SIMS) imaging was used to map lipid distributions across whole brain sections, revealing region-specific alterations in lipid organization associated with disease pathology. In parallel, NanoSIMS enabled high-resolution analysis of protein turnover at the single-cell level, focusing on neuronal populations. This approach allows direct correlation of tissue-level molecular composition with cellular metabolic activity.
Our results demonstrate clear differences in lipid distribution between diseased and control brain regions, alongside measurable changes in protein turnover within individual neurons. These findings indicate that SGS involves concurrent disruption of lipid homeostasis and cellular proteostasis, linking large-scale biochemical remodeling to altered neuronal function.
Together, this study establishes correlative SIMS imaging as a powerful strategy for connecting molecular and cellular changes in neurological disease, providing new insight into the multiscale mechanisms underlying SGS pathogenesis.

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Key words: Schinzel-Giedion syndrome; SETBP1; correlative SIMS; ToF-SIMS; NanoSIMS; lipid homeostasis; protein turnover; neuronal metabolism

Isotope Tracing of Elemental Diffusion in Stainless Steel Oxide Scales for SOFC Applications

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The long-term oxidation resistance of stainless steel connectors is critical for the reliable operation of solid oxide fuel cells (SOFCs), a promising technology for green energy generation. This study employs isotope tracing combined with ToF-SIMS to systematically investigate the oxidation mechanism of T91, 304, 310S, 316LN, and 709 stainless steels after exposure at 700 °C. Results reveal that the oxide scales formed on all steels consist of spinel and Cr_2O_3 layers. However, distinct growth mechanisms were identified: oxide scale thickening in T91 steel is governed primarily by outward cation diffusion, whereas inward anion and outward cation mixed diffusion dominates in 304, 310S, 316 and 709 steel. Notably, the oxide scales on 304 and 709 steels exhibit thin oxide scales, suggesting that the mixed diffusion mechanism promotes enhanced alloys' oxidation resistance. This work clarifies the relationship between diffusion mechanisms and oxidation resistance of oxide scales on the tested stainless steels at elevated temperature, while also demonstrating an effective approach for probing elemental diffusion kinetics during alloy oxidation. The findings are expected to provide valuable guidance for failure analysis of electrode materials in SOFCs.

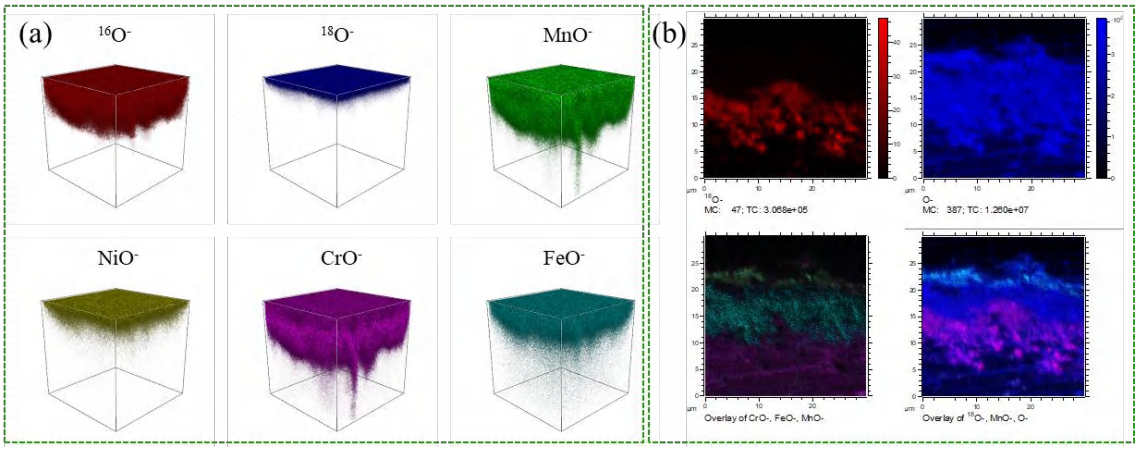


Fig. 1. Elemental distribution of oxide scales formed on stainless steel.(a) 3D isotope oxygen distribution in T91 steel after 5 h oxidation at 700 °C. The oxidation process consisted of two stages: from 0–1 h, the T91 steel was exposed to Ar-20%$^{16}O_2$ mixed gas; from 1–5 h, it was exposed to Ar-18%$^{16}O_2$-2%$^{18}O_2$. (b) Overlay isotope oxygen distribution in 310S steel after 20 h oxidation at 1100 °C. The oxidation process also consisted of two stages: from 0–5 h, the 310S steel was exposed to Ar-18%$^{16}O_2$-2%$^{18}O_2$ mixed gas; from 5–20 h, it was exposed to Ar-20%$^{16}O_2$. Red, blue, green, magenta, and cyan represent $^{18}O^-$, $^{16}O^-$, MnO^-, FeO^-, and CrO^- ions, respectively.

3D Mass Spectrometry Imaging of Multicellular Tumor Spheroid: Cryogenic ToF-SIMS coupled with Argon Gas Cluster Ion

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High-vacuum conditions in conventional ToF-SIMS cause drying artifacts, where water evaporation triggers the migration and aggregation of lipids, distorting their native spatial distribution.[1] To prevent such physicochemical alterations and capture the true molecular architecture of biological systems, maintaining a frozen-hydrated state during analysis is essential.[2]

We established an artifact-free 3D MSI platform by integrating cryogenic ToF-SIMS with Argon Gas Cluster Ion Beam (Ar-GCIB) sputtering. Using 3D SKOV3 ovarian cancer spheroids, we compared air-dried and cryogenic samples. Air-dried samples exhibited severe spatial distortion, with major lipids (e.g., FA 18:1, PI 38:4) migrating to the surface and increasing in concentration by up to 10-fold. In contrast, the cryogenic platform successfully preserved the native lipid distribution from the periphery to the spheroid core. Molecular identities were cross-validated via LC-MS/MS, ensuring high analytical rigor.

This platform preserves the chemical information of the tumor microenvironment in its native state and precisely reconstructs it into a high-resolution 3D molecular map. By effectively eliminating drying-induced artifacts, this approach provides a robust tool for studying spatial lipid metabolism and targeted drug delivery mechanisms in precision oncology.

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Keywords: Mass Spectrometry Imaging, Cryogenic ToF-SIMS, Multicellular Tumor Spheroids, Argon Cluster Sputtering, Lipidomics, Drying Artifacts

Growth and properties of AlF_3 Films on Silicon: Effect of Electron Bombardment

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Due to their high transparency, wide band gap, and passivation properties, AlF_3 films have been proposed to extend the lifespan of silicon electrodes in batteries [1] and as a coating of solar cells, where creating a negative layer near the Si interface requires controlled and localized F-depletion [2]. This work investigates the growth of AlF_3 layers on Si (111) in UHV, and shows that the depletion of F can be induced and controlled by electron bombardment of the film immediately after deposition, as shown previously [3-4]. New MC simulations identify the optimal electron energy relative to film thickness. Film composition and surface smoothness were characterized using XPS, AES, and AFM. TOF-SIMS depth profiling [Fig.1] provides information about thickness, F-depleted regions and potential diffusion into the substrate. Matrix effects, sputtering rates, flood gun influence, and AlF_x cluster formation are discussed.

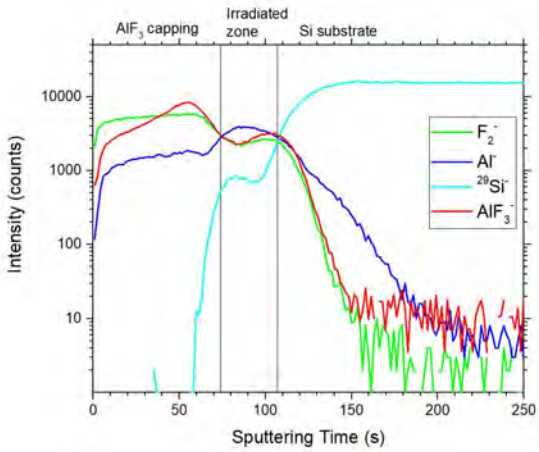


Figure 1. TOF-SIMS depth profiling of a sample consisting of a Si substrate, an AlF_3 layer irradiated with low-energy electrons and a non-irradiated AlF_3 layer for capping.

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Spatial Lipidomics of Prostate Cancer Cells and the Effects of Aspirin using Multimodal Imaging

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Prostate cancer (PCa) is one of the most diagnosed cancers in men, however, management of this disease remains a challenge due to variation in clinical prognosis [1]. Further insight into the structure and behaviour of this disease is needed to improve clinical approaches. There is strong evidence linking PCa progression and lipid metabolism dysregulation, with increasing interest in the COX-2 enzyme and its potential role in tumor metastasis [2]. Evidence suggests that Non-Steroidal Anti-Inflammatory Drugs (NSAIDs), such as aspirin, have anti-tumor properties, with research showing that they can inhibit the COX-2 metabolomic pathway [3]. PCa cells are incredibly heterogenous, which traditional life science techniques fail to resolve. Therefore, the introduction of single-cell analysis is vital in furthering our understanding of the cellular mechanisms of the disease.

In this work, we have used Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) with vibrational spectroscopy techniques, Fourier-Transform Infrared (FT-IR) and Optical-Photothermal Infrared (O-PTIR), to chemically image the spatial lipid profile of PCa cells after treatment with aspirin, including monitoring the uptake and metabolism of arachidonic acid. ToF-SIMS enabled label-free imaging of PC-3 cells, using different cluster primary ion beams to achieve high biological sensitivity and specificity at a single-cell resolution. FT-IR facilitated high-throughput analysis of the same cell populations, supported with data from the sub-micron imaging with O-PTIR.

As part of this work, we addressed the challenges associated with multimodal imaging, such as reproducible sample preparation, measurement and data analysis workflows. We discuss the integration of different chemical imaging modalities and their effective utilization in single-cell analysis, potentially contributing to a better understanding of cellular lipidomics and its role in disease progression.

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Investigating the Effect of Fine Particulate Matter on Human Bronchial Epithelial Cells Using TOF-SIMS and Raman Imaging Techniques

Manale Noun

Air pollution is one of the greatest reasons for premature mortality, with profound implications for the environment and human health. Fine particulate matter (PM) can easily penetrate the respiratory tract, inducing an inflammatory response that initiates and exacerbates multiple respiratory diseases [1].

The objective of this study is to investigate the effects of these particles on pulmonary cell models. Human bronchial epithelial cells (BEAS-2B) were cultured under normal conditions and exposed for 24 hours to different concentrations of SRM2786 standard particulate matter (3, 12, 24, and 96 $\mu g/cm^2$) deposited onto silicon substrates. The cells were subsequently fixed, dried, and analyzed using two complementary imaging techniques: Time-of-Flight Secondary Ion Mass Spectrometry equipped with bismuth and argon clusters sources and confocal Raman microscopy operated with a 532 nm laser. Various computational methods were applied to evaluate these responses.

TOF-SIMS results revealed changes in fatty acid compositions, particularly palmitic, palmitoleic, stearic, oleic, and linoleic acids, as well as amino acid fragments. Two- and three-dimensional distributions of characteristic components from PM, cellular membranes, and nuclei were plotted to further investigate the inflammatory response. Raman spectroscopy showed marked spectral changes associated with DNA, lipids, and proteins consistent with an inflammatory cellular response. Significant decreases were observed in cytochrome-associated bands, reflecting mitochondrial alterations. Protein-associated bands, such as phenylalanine and amide, likewise decreased, consistent with protein carbonylation and structural alterations. Lipid bands exhibited more complex behavior, with decreases in C=C and CH_2 vibrations alongside an increase in CH_3 vibrations, suggesting lipid peroxidation and changes in lipid composition [2-3].

The use of these two complementary imaging techniques provides new insights into the cellular mechanisms induced by PM exposure, improving our understanding of its contribution to respiratory diseases.

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Investigation of lithium transport in Li-ion batteries by isotope tracing using FIB-SIMS

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Higher energy density, longer lifespan and safer units are critical aspects to be considered in the next-generation LIBs. The formation and evolution of the solid electrolyte interphase (SEI), structural changes of the active materials, lithium transport mechanism within electrodes, and loss of lithium during the battery life play a critical role in the degradation and performance loss of the battery. These challenges demand new advanced analytical workflows to facilitate a comprehensive understanding at the nanometer-scale of the physical, chemical, and electrochemical processes during operation [1-2].

FIB-SEM-SIMS platforms equipped with a magnetic sector SIMS system combine in a single instrument Electron Microscopy (i.e. SE, STEM, BSE) with high-resolution SIMS, down to 15 nm [3]. This exceptional resolution enables simultaneous multiscale EM-SIMS imaging across the entire electrode microstructure, from electrode-electrolyte interface through the bulk material to the current collector. Lithium isotopic tracing emerges as a powerful, robust methodology for tracking lithium dynamics at nanometer scale [1]. This approach involves "labeling" lithium-containing components with isotopically enriched lithium (e.g., ^{6}Li or ^{7}Li), allowing these tracers to participate in electrochemical cycling. By analyzing the final isotopic distribution using HR-SIMS, one can precisely map lithium movement, transformation, and sequestration within the LIB.

In this contribution, we applied a specific FIB-based methodology for multiscale post-mortem analysis of LIB electrodes which allows: i) high flexibility to inspect the entire electrode; ii) full electrode depth analysis; iii) simultaneous investigations of interphases and bulk material with the capability to resolve nano-sized constituents [4]. Specifically, in silicon-carbon/graphite negative electrodes with 300 cycles, progressive formation of SEI in the Si-C composite is observed. Isotopic tracing indicates partial lithium trapping in the degraded volume of the particle. This enables direct assessment of local lithium transport properties at sub-particle level. The complementarity of FIB-SIMS with bulk-sensitive techniques such as ss-NMR or ICP-MS was performed to provide comprehensive lithium tracking. This work demonstrates how advanced instrumentation and isotopic tracing can transform battery research, enabling rational design of more durable, safer, higher-performing lithium-ion batteries through mechanistic understanding of lithium dynamics at nanoscale.

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TOF-SIMS Technology for Characterizing Covalently Linked Self-Assembled Bilayer Structures

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Self-assembled monolayers (SAMs) are widely used as electron transport layers in inverted perovskite solar cells due to their low cost, low optical/electrical losses, and tunable energy levels and surface properties. However, their poor thermal stability under high temperature and thermal cycling limits device long-term operation. In this study, a covalently linked self-assembled bilayer (SAB) structure was designed, and a covalently bonded polymer network system was constructed via Friedel–Crafts alkylation reaction. This covalent connection effectively anchors the small-molecule SAM layer on the transparent conductive substrate, synergistically enhancing device photoelectric performance and environmental stability. A power conversion efficiency (PCE) over 26% was achieved, with only slight attenuation during long-term damp-heat exposure and multiple thermal cycling tests[1].

Time-of-flight secondary ion mass spectrometry (TOF-SIMS) is crucial for SAB structure characterization, featuring ultra-high surface sensitivity, near-nondestructive detection, and high mass resolution, which is well-suited for analyzing ultra-thin organic self-assembled layers; using a Bi_3^+ cluster ion source to obtain macromolecular ion fragments, we detected methylene-bridge-linked Friedel-Crafts coupling products by comparing mass spectra of single SAM and modified SAB samples, directly confirming successful SAB construction. This study demonstrates TOF-SIMS' ability to accurately analyze organic layer surface structures, break traditional characterization limitations, provide direct evidence for covalent network formation, and offer a reliable analytical paradigm for high-stability perovskite optoelectronic device design and optimization, as well as its potential in advanced functional material characterization.

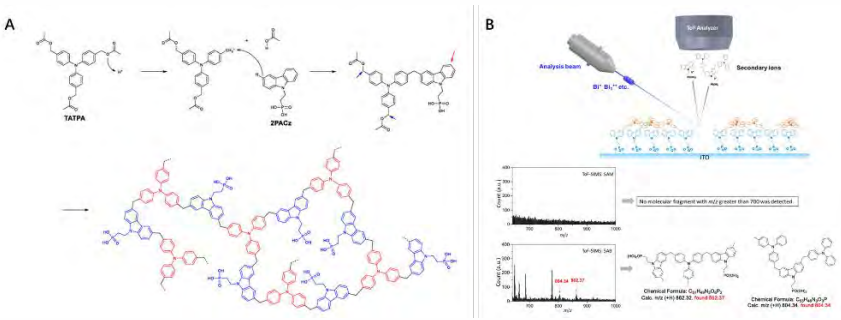


Figure (A). Schematic diagram of SAB structure and formation. Figure (B) . TOF-SIMS results of SAB.

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Microscale Characterization of Composite Decorative Layers in Chenghua Doucai Porcelain by ToF-SIMS

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Doucai porcelain is distinguished by its combination of underglaze blue decoration and overglaze low-fired enamels, and constitutes an important category of composite-decorated ceramics in ancient China. Its visual appearance and coloration are governed not only by the composition of chromogenic elements such as Co, Fe, and Cu, but also by the stratigraphic arrangement, interfacial microstructure, and possible elemental migration among the underglaze blue, transparent glaze, and overglaze enamel layers during successive firing processes. In particular, the manner in which the underglaze blue and overglaze enamels form a decorative system that is structurally distinct yet technically interconnected through the transparent glaze layer remains to be clarified through microscale elemental and interfacial analysis.

To investigate the layer sequence and interfacial relationships among the ceramic body, transparent glaze, underglaze blue decoration, and overglaze enamel layers in Chenghua-period doucai porcelain, this study will employ time-of-flight secondary ion mass spectrometry (ToF-SIMS) for microscale elemental and ion imaging of polished cross-sections. The spatial distributions of chromogenic and flux-related elements, including Co, Fe, Cu, Mn, and Pb, together with major matrix elements such as Si, Al, Ca, K, and Na, will be examined across different decorative regions. By comparing elemental enrichment, diffusion ranges, and interfacial transition features in various decorative units, the study aims to characterize the material composition, stratigraphic structure, and firing-related differences between underglaze blue and overglaze enamel decorations.

Particular attention will be given to the occurrence and distribution of blue colorant elements within the transparent glaze and their association with the glaze matrix. The interface between the overglaze enamel layer and the glaze surface will also be analyzed to identify the material characteristics of low-fired enamels and to assess possible elemental migration or interlayer reactions between the underglaze and overglaze components. Through an integrated analysis of elemental distribution, interfacial transitions, and microstructural differences, this study seeks to establish a microscale structural model for the composite decorative layers of Chenghua doucai porcelain, providing materials-based evidence for understanding its coloration mechanism, decorative sequence, and firing technology.

Keywords: ToF-SIMS; Chenghua period; doucai porcelain; underglaze blue; overglaze enamel; interfacial structure

Self-Supervised TOF-SIMS Formula Assignment via Contrastive Representation Learning on Public Mass Spectral Repositories

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Supervised deep learning holds immense promise for mass spectrometry data analysis, yet its application to TOF-SIMS remains blocked by a fundamental bottleneck: training modern neural networks requires massive labeled datasets, but manually annotating millions of mass spectra with correct elemental formulas is prohibitively expensive. We demonstrate that this barrier can be circumvented by exploiting public mass spectral repositories as a source of free training supervision, combined with contrastive representation learning that ranks candidate formulas in a semantically structured embedding space—eliminating the need for manual annotation entirely [1].

Our pipeline integrates three components into a fully automated workflow. A rule-based engine first performs peak detection and formula enumeration on raw spectra, generating candidate elemental compositions for each observed mass peak. We then leverage the MassBank database—122,512 curated spectra spanning 8,907 unique molecular formulas—to automatically construct training data: matching observed peaks to database entries yields 644,805 additional formula-spectrum mappings and 1.92 million balanced training samples without manual labeling. Finally, a dual-model architecture scores the candidates. A lightweight 1-D Residual CNN (56K parameters) performs multi-label element detection with positive weighting, while a Transformer encoder trained with Triplet Margin Loss learns a contrastive embedding where correct formula-spectrum pairs are pulled together and incorrect ones pushed apart—replacing conventional regression scoring with a structured ranking objective. The architecture is inherently extensible: as public databases expand, new compounds and elemental species are incorporated without architectural modification [2,3].

Validated on 2,840 experimental TOF-SIMS spectra spanning two independent datasets, the pipeline demonstrates consistent multi-label element detection across a broad range of elemental species. The contrastive Transformer learns a discriminative embedding space, attaining a positive-vs-negative cosine similarity gap of 0.014 after training on 318,171 automatically mined triplets—each comprising an anchor spectrum, a correct formula, and a confounder sampled from adjacent mass regions. End-to-end inference yields 405,483 peak assignments at 99.93% spectrum coverage with zero processing failures, confirming robust generalization across diverse sample types without per-dataset tuning [4].

This work establishes a scalable paradigm for analytical mass spectrometry: rather than depending on costly manual annotation, deep learning models can be trained on supervision automatically mined from community databases, and continuously improve as those repositories grow. The pipeline achieves formula-assignment breadth and accuracy previously attainable only through extensive expert curation, while its modular design ensures that expanding elemental coverage requires no architectural changes—only additional database entries. We are currently extending the framework to incorporate isotopic fine-structure analysis and preparing an open-source release to facilitate community adoption and collaborative development [5].

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New results with cryo introduction on the NanoSIMS-HR

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The NanoSIMS-HR, introduced in March 2024, is the successor of the NanoSIMS 50L and incorporates major technological advances, particularly for Cs^+ primary ion analysis. Key improvements include enhanced lateral resolution down to 30 nm, depth resolution of 12 nm per decade, push-button remote automation of sample holder handling and exchange, and an ultra-precise sample stage that increases navigation efficiency and enables up to a 10xfold faster throughput during unattended, chained analyses. The instrument also integrates a cryogenic stage, enabling the analysis of samples introduced at room temperature. After loading, samples are cooled and frozen *in situ*, allowing them to be analyzed as solid materials. This capability was demonstrated through isotopic measurements of fluid inclusions trapped in chert, achieving precisions of ±16‰ (1 SD) for hydrogen and ±4‰ (1 SD) for oxygen isotopic ratios.

In this conference, we introduce a new cryogenic sample introduction capability for the NanoSIMS-HR. This accessory enables direct loading of cryogenic samples prepared using a controlled cryo workflow, from quenching in liquid nitrogen through cryogenic coating and finally transfer to NanoSIMS for imaging under cryogenic conditions. We present recent imaging results obtained on cryo-prepared emulsions and biological samples. This cryogenic introduction system is available as an accessory and can be installed on any NanoSIMS-HR instrument.

Development of a Three-Dimensional Reconstruction Workflow for Serial ToF-SIMS Imaging Data of Brain Tissue

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ToF-SIMS imaging provides molecular information from biological tissues, but data acquisition is inherently limited to two-dimensional sections. This limitation makes it difficult to evaluate the spatial relationships of molecular signals across consecutive anatomical positions in structurally complex and heterogeneous organs such as the brain. In this study, a three-dimensional reconstruction workflow was applied to serial ToF-SIMS data from SD rat brain to integrate multiple lipid-related ion signals within a unified spatial framework.

Serial coronal sections were collected with a thickness of 10 μm and a sampling interval of 500 μm. For each section, signal-positive pixels were retained by threshold-based filtering and converted into spatial points according to their in-plane coordinates and section index. The resulting point-cloud slices were then assembled along the sectioning axis using interpolation, and H&E-guided rigid alignment was applied to improve spatial consistency across sections.

The reconstructed volumes revealed distinct spatial patterns among lipid-related ions in the SD rat brain, as shown in Figure 1. Cholesterol exhibited a more localized and structured distribution, whereas phosphocholine and choline showed broader tissue coverage while retaining clear anatomical organization. The vitamin E-related ion displayed weaker and more discontinuous signals. These results indicate that serial ToF-SIMS data contain ion-specific spatial information that is difficult to capture from individual two-dimensional sections. By combining whole-brain reconstruction, ion-overlay visualization, and ROI-based analysis, this workflow provides a practical framework for describing molecular heterogeneity across global and local anatomical scales and extends ToF-SIMS analysis toward spatially integrated molecular mapping.

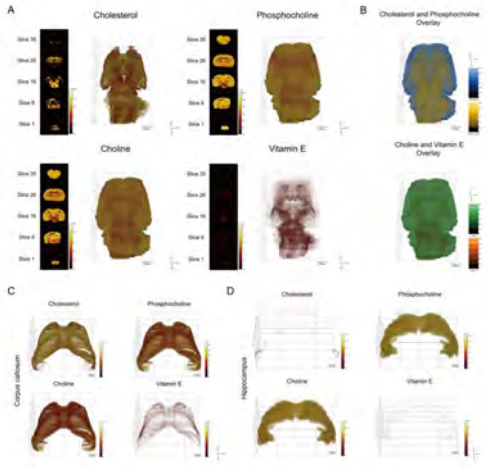


Figure 1. Three-dimensional reconstruction of lipid-related ion distributions from serial ToF-SIMS brain-tissue images.

Observation of topography development on Si surface caused by oblique incident O_2^+ ion beam over a range of ion parameters

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Surface rippling on Si by oblique incident O_2^+ ion beam is a well-known phenomenon [1,2] though there seems to be no satisfactory theory of its mechanism. Aiming to provide a set of detailed experimental results which might contribute to verification of theories of rippling mechanism, we observed Si(100) surface topography by atomic force microscopy (AFM) over a range of ion energy E:0.5-3keV, angle of incidence θ:10-75deg and ion dose:0-1.5E19 ions/cm^2. The observed topography was categorized according to its appearance and 2-dimensional power spectral density (2DPSD). Though Ar^+ sputtering was reported to show a boundary between "flat-" and "ripple-" zones at θ=48deg [3], O_2^+ sputtering showed the boundary at θ=30-45deg depending on E. We will show the variation of 2DPSD, ripple wavelength λ and roughness with the ion parameters.

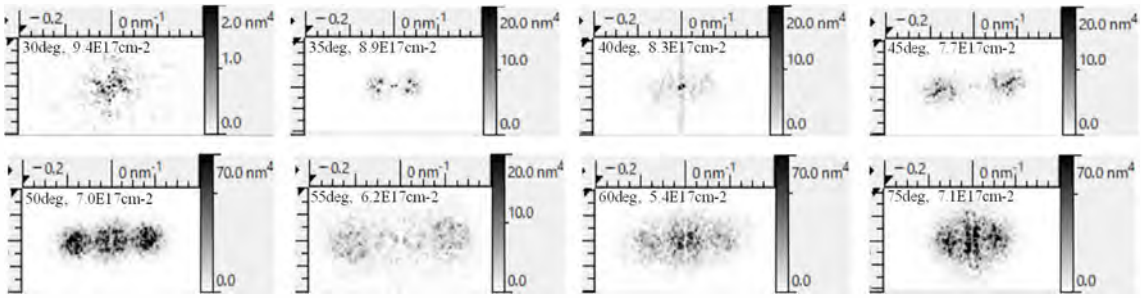


Figure 1. Typical variation of 2DPSD with θ at low dose levels (E=2keV)
θ and ion dose are shown in each 2DPSD.

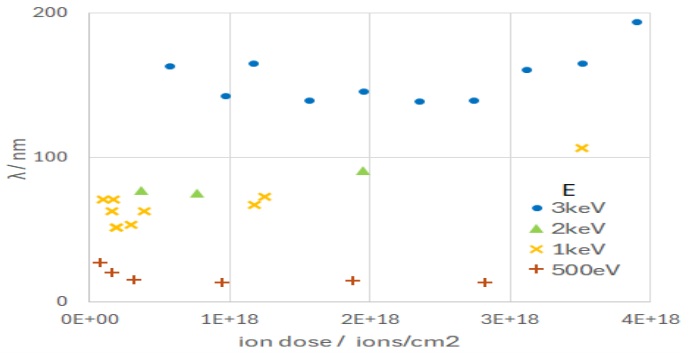


Fig.2 Examples of λ variation with ion dose at θ=45deg.

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TOF-SIMS Characterization of Uranium Binding to Carboxylic-Acid-Functionalized Phenoxycalix[4]pyrrole

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Uranium is a naturally occurring radioactive and chemically toxic heavy metal whose recovery and removal from aqueous environments remain strategically important for environmental protection, nuclear-resource sustainability, and long-term energy security. Although seawater contains uranium at very low concentrations, its enormous volume makes it an attractive reservoir, provided that selective and efficient extraction materials can be developed. Phenoxycalix[4]pyrrole (PCP) based supramolecular receptors are attractive candidates for uranyl capture because their molecular cavity and tunable pendant arms can be functionalized to improve metal-ion recognition. Among PCP and its two functionalized derivatives, ester-functionalized PCP1 and carboxylic-acid-functionalized PCP2, the latter was identified as the most promising receptor for uranium extraction. This behavior is attributed to the presence of carboxylic-acid groups, which provide oxygen-donor sites favorable for uranyl coordination. Under optimized conditions, PCP2 reached up to 85.93% uranium extraction [1].

TOF-SIMS characterization was performed on uranium loaded PCP2 powder samples to identify uranium-containing secondary ions associated with the receptor after extraction. The spectra revealed the deprotonated molecular ion of PCP2, confirming preservation of the ligand molecular signature, while the detection of uranium containing secondary ions assigned to PCP2–uranyl associated species supported uranium binding on the extracted material. Proposition: TOF-SIMS analyses were further carried out on PCP2 samples collected after uranium extraction under different experimental conditions, including those from Doehlert optimization, different uranium concentrations, and varying extraction times. The TOF-SIMS results were discussed in relation to gamma-spectroscopy data and showed comparable global trends, with stronger uranium-related signals observed under conditions associated with higher uranium uptake. Additional TOF-SIMS investigations were also carried out to assess material recyclability by following the persistence or decrease of uranium-related signals after reuse cycles.

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Ice deposition from Water Gas Cluster Ion Beams ((H2O)n+-GCIB) at cryogenic temperature

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Water Gas Cluster Ion Beams ($(H_2O)_n^+$-GCIB) have been proven as an excellent primary ion beam in secondary ion mass spectrometry (SIMS). Especially in biological sample imaging, it helps reducing fragmentation of biological molecules, improves ionisation efficiency, while maintaining 1-2 mm spatial resolution. Meanwhile, acquisition of SIMS datasets at cryogenic temperature shows some unique advantages. It has been observed that cryogenic temperature enhances ionisation of biomolecules and thus facilitates their detection. In addition, maintaining biological samples at cryogenic temperature will also facilitate potential correlative imaging with electron microscopy (EM), where preserving the near-native state of the samples is crucial.
Here we explore one of the obstacles in $(H_2O)_n^+$-GCIB-SIMS at cryogenic temperature: ice deposition on the targeted surface. This continuous ice deposition can gradually stop the primary $(H_2O)_n^+$-GCIB reaching the surface, making further depth profiling impossible. We identify the type and source of the ice deposition and studied multiple characteristics of this phenomenon. Our aim is to provide a clearer picture of the phenomenon, the impact of it, as well as the potential approaches to minimise it.

Key words: cryogenic, water, ion-solid interactions, cluster ion beams

Application of Time-of-Flight Secondary Ion Mass Spectrometry in Fingerprint Analysis

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Time of Flight Secondary Ion Mass Spectrometry (ToF-SIMS) has the advantages of high spatial resolution, high mass resolution, non-destructive, and parallel analysis. It is a static SIMS surface analysis technique suitable for elemental, inorganic, and organic analysis of solid surfaces. Therefore, in the field of fingerprint analysis applications, it can provide information for fingerprint analysis and applications from two dimensions: macro to micro, and from major components to trace components. This study investigated the use of ToF-SIMS in tertiary fingerprint features, demonstrated the enhanced analysis of residual fingerprints on Chinese yuan（RMB） using ToF-SIMS, and demonstrated its application in identifying the authenticity of blood fingerprints.

Synergies of ToF-SIMS Analysis and SPM Techniques

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Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) and Scanning Probe Microscopy (SPM) are complementary measurement techniques for surface characterisation. Combining both leads to more conclusive and reliable findings, while in-situ measurements improve the quality and comparability of the results.

Elemental and molecular chemical information is obtained by ToF-SIMS. Although this extremely sensitive analysis technique is inherently destructive, it does not affect itself within the limits of static SIMS, as the induced surface damage is negligible. Applying a focused primary ion beam lateral surface structures down to a few tens of nanometers can be chemically resolved.

Scanning Probe Microscopy (SPM) resolves surface structures on the nanometer-scale, in the most prominent mode by measuring the surface topography. Furthermore, advanced SPM modes allow measuring mechanical and electrical properties of the sample such as elasticity, conductivity or work function. SPM is usually a non-destructive method. The underlying contrast mechanism is based on the direct interaction between the probing tip and the sample surface.

Beyond the obvious and proven combination of topography measured by SPM and the chemical map or depth profile of the ToF-SIMS, also other correlated measurements are possible using an *in-situ* combination instrument. One example demonstrated in this presentation is the assessment of electrical properties by SPM and its correlation to the chemical composition revealed by ToF-SIMS.

Besides analytical applications, also fundamental insights are provided by combining these methods. The ion bombardment during ToF-SIMS analysis affects the electrical properties of the sample, which are measured with SPM. On the other hand, the electrical properties of the surface strongly influence the ion formation in SIMS. Already for dose densities significantly below the static limit, variations in the work function can be observed by SPM. Systematically investigating this and similar effects can be used to better understand the ionisation process in SIMS.

Topography-Tolerant Chemical Mapping of Coatings Using Cluster SIMS for Failure Analysis of Electronic Components

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Cathodic delamination of organic coatings on electronic components, including printed circuit boards (PCBs), and the subsequent galvanic and electrochemical corrosion, represent critical reliability failures in the electronics industry. Time-of-flight secondary ion mass spectrometry (ToF-SIMS) is a powerful analytical technique for the chemical characterisation of such coatings. However, conventional instruments employing a pulsed primary ion beam suffer from several measurement artefacts when applied to geometrically complex samples. These include shadow effects arising from protruding structures, topography-induced matrix effects caused by variations in local surface angle, and charge build-up on insulating organic coating surfaces. Collectively, these artefacts render direct measurement of as-received electronic components unreliable.
To mitigate these limitations, cross-sectional sample preparation is commonly employed, whereby the component is sectioned to expose a nominally flat surface for analysis. However, this approach introduces a significant risk of surface contamination during the cutting and polishing process. Such contamination may adhere to the region of interest, obscuring the very chemical features that the analysis seeks to resolve, and thereby compromising the integrity of the resulting data.
Our Cluster SIMS (J Series III, Ionoptika Ltd.) overcomes these challenges through two key design features: secondary ion pulsing, rather than primary ion pulsing as used in conventional ToF-SIMS, and an extended extraction gap of 8 mm between the analyser and the sample surface rather than 1.5 mm. This configuration substantially reduces the influence of surface topography on measurement accuracy, enabling reliable chemical analysis of samples with complex three-dimensional geometries without the need for cross-sectional preparation.
In this work, the spatial distribution of coating materials within recessed features of geometrically complex electronic components was measured directly using the J Series III Cluster SIMS. Coating distribution data with markedly reduced topographic artefacts were successfully obtained. Chemical mapping of the coating surface enabled clear visualisation of the root causes of component failure, specifically corrosion initiation and coating delamination, in regions that would otherwise be inaccessible or compromised by conventional sample preparation.
These findings demonstrate that the Cluster SIMS not only simplifies the sample preparation workflow but also eliminates secondary contamination introduced by handling during cross-sectioning. This suggests that more accurate, representative, and contamination-free chemical data can be acquired from electronic components with complex surface geometries, with direct implications for failure analysis and quality assurance in electronics manufacturing.

Characterization of Hyaluronic Acid Nanometric Layers Using ToF-SIMS

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Hyaluronic Acid (HA) coatings on Polyvinyl Chloride (PVC) are widely used in medical devices to improve biocompatibility and surface lubrication. In PVC-based catheters and other implantable or blood-contacting devices, HA coatings can improve patient comfort and reduce tissue damage during insertion and use. Therefore, characterization of the HA layer integrity and uniformity is essential for device reliability and performance.

Time-of-flight secondary ion mass spectrometry (ToF-SIMS) provides high-resolution chemical analysis for samples where Energy-Dispersive X-ray Spectroscopy (EDS) and other usual Electron Microscopy (EM) techniques struggle to find a good compromise between sample preparation and interference with surface chemistry. Trace elements detection and spatial resolution to characterize nanometric layers also present a challenge for EM techniques that are easily overcome with a cluster SIMS system. IONOPTIKA J105 cluster-ion ToF-SIMS was used to perform depth profiling using a $C60^{+}$ primary ion beam in PVC film coated with a nanometric layer of HA. Fig 1 a) shows normalized intensity depth profiles for HA and PVC -related secondary ions. After the surface contamination is removed, we observe a layer with reduced Cl ions and increased Na and K ions that we attribute to the HA layer. In Fig b) and c) we present a map for Na2H+ (b) and C2H4Cl+ (c) intensity at layer #30; showing a hole in the HA layer where PVC is exposed, revealing that the HA layer has defects that can result in device failure. These preliminary results underscore the importance of ToF-SIMS in the design of Bio-compatible structures, as a unique tool that can help sort out key device issues and performance.

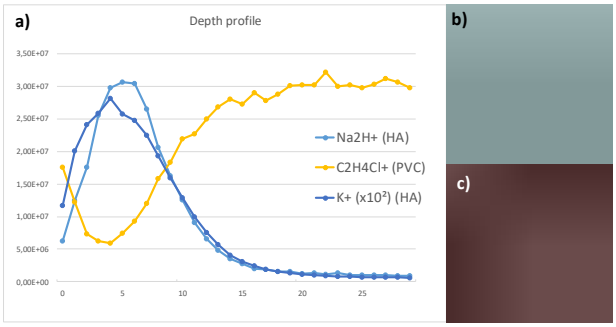


Figure 1. a) Depth profiles for secondary ions species associated to HA and PVC. Secondary ions intensity map for b) Na2H+ and c) C2H4Cl+ mass spec peaks.

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Exploring Dynamic Electrode-Electrolyte Interfaces via Pore-Confined In Situ ToF-SIEMS

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One of the central challenges in investigating electrochemical reactions at electrode-electrolyte interfaces (EEIs) is the precise identification of trace electrogenerated products, transient intermediates, and solvated species, which are often obscured in conventional homogeneous systems. In situ time-of-flight secondary ion electrochemical mass spectrometry (ToF-SIEMS) has emerged as a powerful strategy, offering inherent high mass and spatiotemporal resolution to probe the dynamic evolution of both electrode surfaces and interfacial species.

In this work, we developed an in situ pore-confined ToF-SIEMS technique to revisit the classic electrochemical redox of ferricyanide on a gold electrode under operando conditions. A dynamic potential-dependent behavior of $Au(CN)_2^-$, which correlates closely with the ensemble current response, indicating that the gold electrode participated in the electrochemical redox conversion of $[Fe(CN)_6]^{3-}$ and $[Fe(CN)_6]^{4-}$. This study demonstrates the promising capability of in situ ToF-SIEMS to uncover hidden reaction pathways and molecular-electrode interactions at the EEIs.

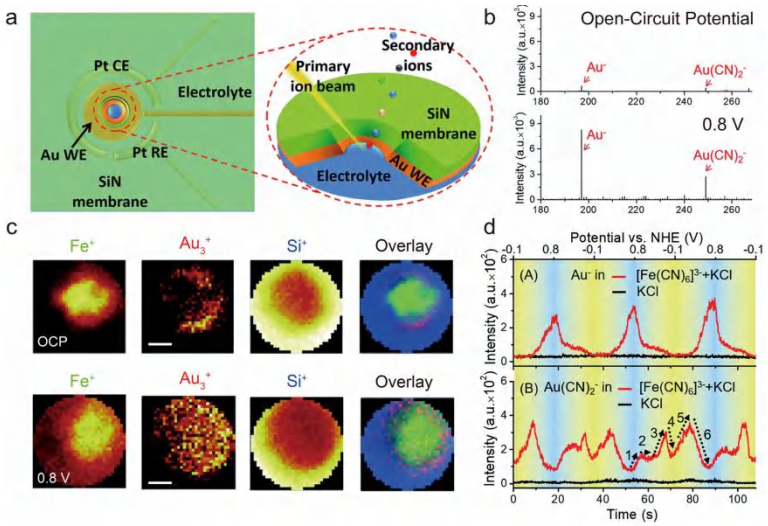


Figure 1. Concept of ToF-SIEMS probing the EEIs through the pore confined configuration.

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Study of EV-Mediated Nucleic Acid Dynamics Using Halogen-Labeled Nucleic Acids

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Extracellular vesicles (EVs) mediate intercellular communication and are involved in various biological processes. Understanding their cellular uptake and intracellular dynamics is essential to clarify their mechanisms. We have previously visualized intracellular DNA and RNA distributions and quantified RNA in EVs using halogen-labeled nucleic acids[1]. Here, we evaluated the distribution of halogen-labeled DNA and RNA derived from EVs by secondary ion mass spectrometry (SIMS) and estimated the required incorporation levels based on sensitivity analysis.

PANC-1 cells were cultured for 48 h in medium containing bromine-labeled RNA substrates. EVs were isolated from the supernatant by size-exclusion chromatography and added to cultured cells for 8 h. Cells were then fixed, embedded, sectioned, and analyzed by SIMS. Sensitivity of bromine was evaluated using embedding resin containing tetrabromobisphenol A (6.8 and 66.2 wppm (weight ppm) Br). SIMS measurements were performed using a NanoSIMS 50L with a 16 keV Cs^+ primary beam.

As shown in Figure 1, bromine signals were localized in the nucleus and mitochondria of cells cultured with Br-labeled RNA. In contrast, cells cultured with EVs showed signal intensities comparable to controls, indicating no detectable bromine from EVs. Based on the sensitivity factor, the background corresponds to ~ 10 wppm, suggesting that ~20 wppm intracellular Br is required for detection.

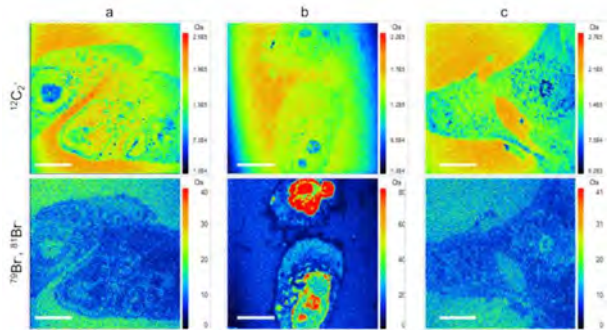


Figure 1. Secondary ion images of control cells (a), cells cultured with Br-labeled RNA (b), and cells cultured with EVs (c), scale bar: 10 μm

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Toward reliable nano-SIMS quantification of residual elements in steel

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The steel industry is undergoing a major transition toward low-carbon production routes based on electric arc furnaces and increased use of steel scrap. Depending on its quality, steel scrap contains 85–98 wt.% iron, while the remaining fraction consists of alloying elements and impurities, including residual elements (RE) that cannot be efficiently removed during steelmaking. Even at low concentrations, RE can significantly affect phase transformations, microstructures and final mechanical properties, making their control a major scientific and industrial challenge.

Understanding the nanoscale distribution and partitioning of RE is therefore essential to predict their impact on steel behaviour. This requires analytical techniques combining high sensitivity with high spatial resolution. Among these techniques, nano-SIMS shows strong potential, although robust methodologies for the quantification of RE in complex steel microstructures are still lacking.

This work investigates the capabilities of nano-SIMS for the qualitative and quantitative analysis of RE in steels. Diffusion couples prepared from pure iron and Fe alloys doped with different RE (Sn, Sb, As and Cu, <0.1 wt.%) were used as reference materials. Concentration gradients characterized by electron probe microanalysis and hardness measurements were used to optimize nano-SIMS analytical conditions and to determine detection limits and sensitivity factors required for reliable quantification of the investigated elements.

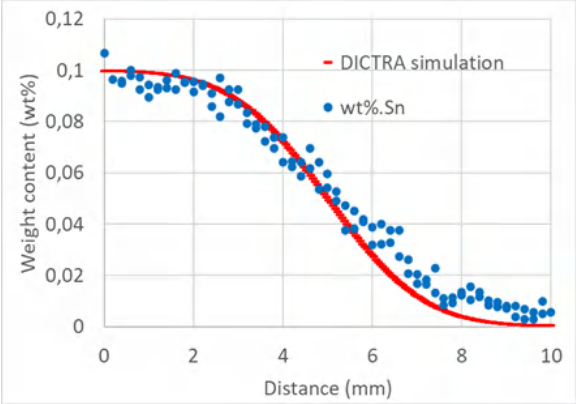


Figure 1. Concentration gradient in a diffusion couple.

This work was supported by the Luxembourg National Research Fund (FNR) through the BRIDGES RESteel project (BRIDGES/2025/MS/19629804).

ToF-SIMS for Cast Iron Characterization

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The performance of steels and cast irons in demanding applications is strongly influenced by microstructural and chemical heterogeneities developed during solidification, thermomechanical processing, and heat treatment. Local segregation of alloying elements and impurities can significantly affect phase stability, precipitation behavior, corrosion resistance, mechanical properties, and susceptibility to environmentally assisted degradation mechanisms, including hydrogen embrittlement [1]. Although conventional characterization techniques provide valuable information on microstructure and bulk chemical composition, the spatial distribution of alloying elements at the micrometer and sub-micrometer scales remains insufficiently understood in many engineering alloys. This limitation is particularly relevant for cast irons and advanced steels, where complex microstructures contain multiple phases, interfaces, graphite particles, eutectic regions, and segregation bands that may locally alter material performance.

Time-of-Flight Secondary Ion Mass Spectrometry (ToF-SIMS) offers unique capabilities for high-sensitivity chemical imaging, enabling the visualization of elemental and molecular distributions with high spatial resolution. The technique is especially attractive for investigating chemical segregation patterns and interfacial chemistry that are difficult to detect using conventional approaches. This enables the statistically representative characterization of segregation patterns in complex microstructures, like the ones shown in Figure 1, for the cast iron sample investigated in this work. By providing high-sensitivity, high-resolution chemical maps, the technique allowed direct observation of segregation patterns for Mn, Cr, Ce, and other elements that directly influence the material phase stability, microstructure and corrosion behavior.

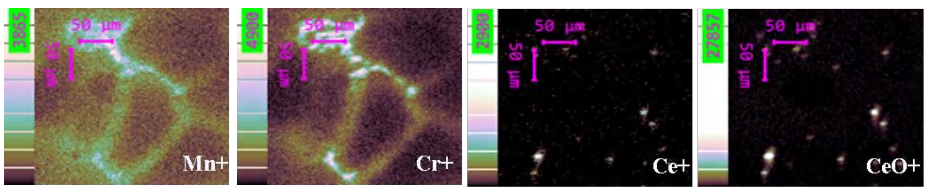


Figure 1. Intensity maps for Mn+, Cr+, Ce+ and CeO+ mass peaks.

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Optimization of Useful Ion Yield for Uranium Particles in LG-SIMS Multi-collection Mode and Preliminary Investigation of ThO^+ Signal Characteristics for Age Dating

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Large-geometry secondary ion mass spectrometry (LG-SIMS) is a core instrument for isotopic analysis and age dating of uranium particles in nuclear safeguard applications [1]. In this work, IRMM-2329P standard uranium particles were adopted to determine the useful ion yield of uranium on vitreous carbon planchets using an IMS 1300-HR^3 LG-SIMS operated in multi-collector mode. The influences of raster size and primary ion beam current under Gaussian mode were systematically investigated. Hydrothermally synthesized uranium oxide particles were further used to compare the effects of four types of primary ion beams (O_2^+, O^-, O_2^-, O_3^-) and two substrate materials (vitreous carbon and silicon) on uranium useful ion yield.

The measurement results show that a 20 μm raster size achieves a well-balanced performance in signal collection efficiency, measurement repeatability and single-particle selectivity, collecting more than 90% of total ion counts even at a beam current of 50 nA. Under identical primary ion conditions, the uranium useful ion yield on vitreous carbon is approximately 30%–40% higher than that on silicon, and negative oxygen ion beams outperform positive beams in ionization efficiency. Among all tested beams, the O_3^- primary beam provides the most prominent improvement in yield. The useful ion yield directly determined with IRMM-2329P certified particles under conventional O_2^+ beam is 2.03%; scaled by relative total U^+ ion counts, the O_3^- beam delivers the highest estimated yield of 3.27% on vitreous carbon, 61% higher than that of O_2^+.

In addition, using thorium nitrate and CRM U850 powder, we preliminarily investigated the signal characteristics of the ThO^+ molecular ion for potential application to uranium particle age dating, with ThO_2^+ evaluated for comparison. Under O_2^+ primary beam and vitreous carbon substrate, ThO^+ exhibits higher signal intensity and better stability than Th^+. With increasing surface oxygen coverage, the signal intensity of ThO^+ can reach more than four times that of Th^+. These findings provide fundamental data on ThO^+ ionization behavior for the development and optimization of uranium particle age-dating methods.

Keywords

particle analysis; uranium particles; LG-SIMS; useful ion yield; nuclear safeguards; ThO^+

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Deciphering Three-Dimensional and Atomically-Dispersed Microstructures of Ion Channels in Deep-Sea Snails

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Deciphering the microstructures and physicochemical properties of marine organisms is crucial for elucidating biomineralization mechanisms in deep-sea environments and developing advanced biomimetic materials, which have not been systematically investigated. In this study, we report on the deep-sea snail *Gigantopelta aegis* (G. aegis), which inhabits the bathypelagic zone at a depth of 2785 meters. This organism exhibits sulfidic biomineralization facilitated by atomically-dispersed iron within an organic matrix, forming channel-like structures in its shells. These features were observed using time-of-flight secondary ion mass spectrometry (ToF-SIMS) and aberration-corrected transmission electron microscopy (ACTEM). Three-dimensional ion channel structures within the snail shell, composed of iron and proteinaceous organic matrices, were evidenced by 3D images reconstructed from ToF-SIMS depth profile results, providing high depth and spatial resolution. ACTEM revealed that iron atoms are individually dispersed as single atoms on a semi-transparent organic substrate. The formation of atomically-dispersed iron is attributed to the ultra-high hydrostatic pressure of the deep sea, which reduces the critical Gibbs free energy, and the organic matrix, which stabilizes the highly dispersed atoms in this chemically dynamic environment[1]. By combining microstructural characterization, we verified the synergistic effect of stabilizing the atomically-dispersed metal and the nucleation process for crystal growth, further elucidating the atomic biomineralization mechanism of iron sulfide in deep-sea snails.

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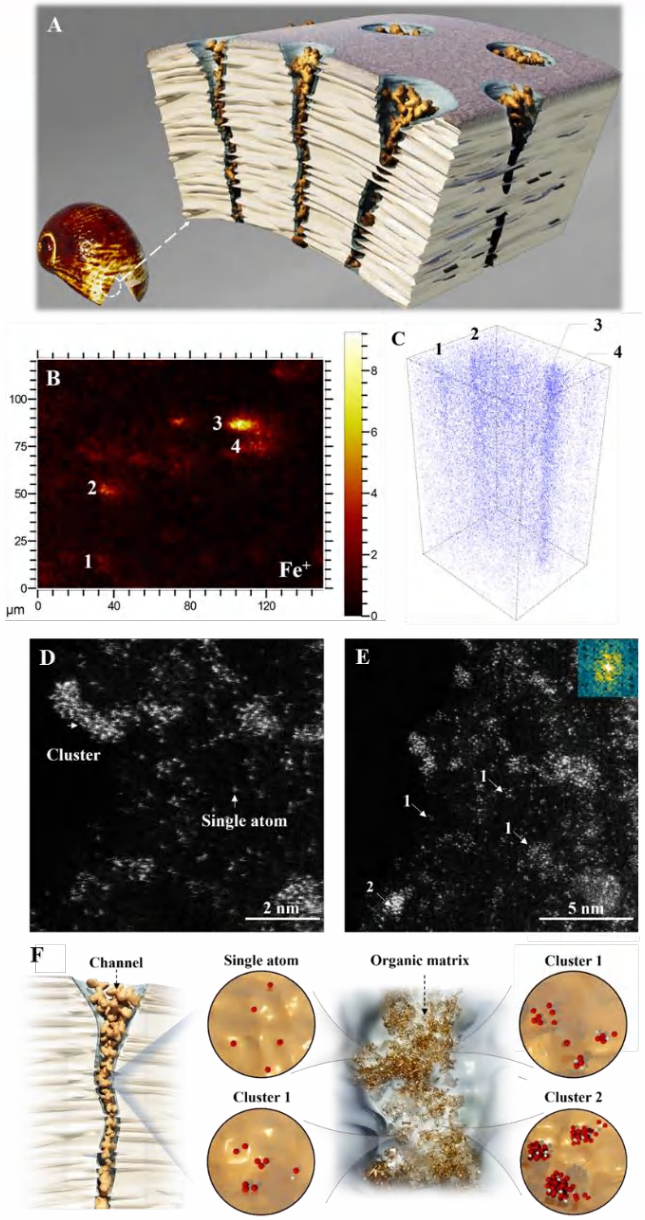


Figure 1. (A) Schematic illustration of ion channel structures in deep-sea snails. (B) 150 × 120 μm ToF-SIMS ion image of the Fe^+ peak at *m*/*z* 55.85 within four ion channels of the snail shell reveals Fe^+ ion accumulation of within the depth of 100 nm of snail shells. (C) 3D images reconstructed from ToF-SIMS depth profile experiments showing the in-depth spatial distributions of Fe^+ (in blue) in positive ion mode within the depth of 100 nm of snail shells. (D, E) High-angle annular dark-field scanning transmission electron microscopy (HAADF-STEM) images of single iron atom and iron clusters on the organic matrix. The inserted FFT analysis was acquired on cluster 2. (F) Schematic illustration of different degree of dispersion morphologies of iron sulfide species on the organic matrix.

Surface Analytical Study of the Electron-Induced Cross-Linking of Molecular Layers into Carbon Nanomembranes

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Carbon nanomembranes (CNMs) [1] are a molecular-thin, carbon-based 2D-sheet material. Their properties (amongst others dielectric, easy chemical functionalisation, intrinsic porosity, ...) are more comparable to ultrathin polymer films than to the complementary and better known 2D material graphene. CNMs are produced by electron beam-induced cross-linking of thin layers of aromatic molecules. Applications of CNMs have been demonstrated in sensor technology [2], energy technology, semiconductor production and especially in filtration and separation (e.g. water filtration membranes [3] for forward osmosis or the provision of ultrapure water). A variety of production methods are possible – from large-area CNM composite membranes for industrial-scale filtration and coatings for modifying various types of surfaces (metals, semiconductors, polymers, etc.), to CMOS-compatible integration even as free-standing nanometre-thin 2D-layers into components. Recently, the roll-to-roll (R2R) production of CNMs on various flexible substrates has been demonstrated by combining vacuum low-temperature evaporation (VLTE) for the deposition of molecular-thin layers of aromatic precursor molecules and low-energy electron irradiation for cross-linking in one industrial-size R2R-coater. Traditionally, self-assembled monolayers (SAMs) of small-sized precursor molecules (e.g. biphenyls) have been used for CNM-production. However, the vacuum-deposition of the precursor molecules enables the use of larger precursor molecules like aromatic polymers, which offers more options to tune the properties of the final CNM.

In this work we used surface analysis, especially ToF-SIMS and XPS, to study the cross-linking process of different precursor molecules – from forming first bonds between the precursor molecules up to fully cross-linked amorphous carbon layers, i.e. a CNM. Whereas the cross-linking process of SAMs of small aromatic molecules is well understood [4], ToF-SIMS and XPS offer new insights into the cross-linking of less densely packed layers of larger molecules. For ToF-SIMS, we chose different primary ions like Bi_1, Bi_3 and Ar-clusters with their different information depth along with various sputter approaches. Thus, we could clearly identify the formation of first bonds between the precursor molecules at the beginning of the cross-linking process. The data showed that even at a relatively low cross-linking density, where ToF-SIMS could still identify the original structure of the precursor molecules, the formed layers were strong enough to be handled as free-standing 2D-sheet materials. This finding is in contrast to experiences with SAM-based CNMs, where a near saturated cross-linking is mandatory for the formation of free-standing 2D-sheets.

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Orbi-SIMS Imaging of Leaf Tissue Sections for Analysis of Agrochemical Penetration

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Understanding the depth-wise penetration and distribution of agrochemicals applied to leaf surfaces is crucial for their research and development. Mass spectrometry imaging (MSI) of leaf tissue sections provides valuable insights into these processes. In this study, we present an optimized method for preparing leaf tissue sections suitable for MSI and demonstrate Z-directional visualization of agrochemical penetration using a secondary ion mass spectrometer equipped with an Orbitrap mass analyzer (Orbi-SIMS).

Potato leaves were treated with either formulation A or formulation B. After 24 hours, treated areas were excised into small pieces. Samples were embedded in Super Cryo-Embedding Medium and rapidly frozen in a dry-ice hexane slurry. Cryo-sectioning was performed using a cryostat (Leica Microsystems, Germany). For improved sectioning quality, cryo-film (SECTION-LAB, Japan) was applied to the leaf surface prior to sectioning. The sections were freeze-dried before MSI. MSI was conducted using an M6 Hybrid SIMS instrument (IONTOF GmbH, Germany), equipped with both a time-of-flight analyzer and a Q Exactive™ Orbitrap mass analyzer. To evaluate detection limits, a dilution series of each formulation was analyzed to determine the minimum detectable concentration.

SEM observations revealed that potato leaf sections thaw-mounted on ITO glass, as well as those mounted on cryo-film without freeze-drying, suffered structural damage due to vacuum-induced water loss. In contrast, combining cryo-film with freeze-drying preserved the native structure of the leaf tissue. The detection limit study demonstrated that Orbi-SIMS enabled more sensitive detection of both formulations on potato leaves compared to TOF-SIMS. This improvement is attributed to differences in ionization efficiency between primary ion species, as well as superior mass resolution and accuracy. Moreover, MSI using the TOF/Orbi-SIMS system revealed that only Orbi-SIMS detected the difference of penetration between A and B : Formulation A showed internal distribution within the leaf, whereas Formulation B remained on the leaf surface. This finding was consistent with the results from the bioassay conducted using leaves and plant pests.

Age Dating of Trace Uranium Particles by Small-Geometry Secondary Ion Mass Spectrometry

Zhong Ningjie[1], Shen Yan[1], Hu Ruixuan[1], Zhao Yonggang [1]

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Age analysis of uranium-containing particles is of great significance in nuclear safeguards and nuclear forensics. The timing of nuclear activities can be traced by measuring the isotopic ratios of uranium and its daughter nuclides [1-4]. In this study, SIMS was used to develop an age analysis method for uranium-containing particles. The relative sensitivity factors (RSFs) of uranium (U) and thorium (Th) were determined, measurement conditions were optimized, standard reference material (CRM) particles with different abundances and particle sizes were analyzed for age dating, and the measurement method of thorium oxide ions (ThO^+) was explored to improve detection sensitivity. The results show that the relative sensitivity factor of U and Th is 1.26±0.05. The optimized SIMS method can accurately determine the age of uranium-containing particles with particle size ≥2.6 μm and abundance ≥20%, with internal precision better than 20% and relative error less than 15%. Furthermore, gallium arsenide substrate combined with oxygen flooding technology can lower the detection limit for age measurement by enhancing the ThO^+ signal. This study provides a reliable method for age analysis of trace uranium-containing particles in the field of nuclear safeguards and possesses important application value.

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Thyra: Native Conversion of Mass Spectrometry Imaging Data into the SpatialData Ecosystem

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Mass spectrometry imaging (MSI) maps the molecular composition of biological samples, and ToF-SIMS extends this to subcellular detail. Yet MSI data remain isolated from the rest of spatial biology. Every instrument writes its own format, and the community standard imzML struggles with modern data volumes and has no place for microscopy or other spatial omics data. Each modality therefore stays in its own software, out of reach of the analysis methods developed for spatial omics.

We present Thyra [1], an open-source Python library that converts MSI data directly into the SpatialData framework [2], a scalable ecosystem for multimodal spatial omics. Thyra reads vendor formats and imzML and writes one open store that is loaded lazily and queried spatially. We first demonstrated it on glioblastoma sections, combining MALDI-MSI lipidomics with Xenium spatial transcriptomics measured on the same tissue [3].

Here we show that ToF-SIMS data integrate in the same way. Thyra reads the raw event stream of a PHI nanoTOF acquisition without an intermediate export, keeps the pixel size recorded by the instrument, and places the spectra on a mass axis that follows the peak width of the analyser. For a tissue section imaged at 1 µm pixel size (512 × 512 pixels, 18.4 million ion events), the converted total ion image is identical, pixel for pixel, to the image exported by the instrument software. Once in SpatialData, the data need no SIMS-specific software. Ion images and multi-ion overlays are drawn with spatialdata-plot, and the pixel spectra pass through the standard spatial omics tools scanpy and squidpy for clustering, embedding and neighbourhood analysis. Microscopy images and other omics layers of the same sample can be stored in the same object, in a shared coordinate framework, which prepares ToF-SIMS for multimodal studies. By bringing SIMS, MALDI and spatial omics into one open format, Thyra gives the SIMS community access to a rapidly growing analysis ecosystem.

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