



# PTM2022

## The 8th International Conference on Solid→Solid Phase Transformations in Inorganic Materials

June 27<sup>th</sup>- 30<sup>th</sup>, 2022 Virtual Meeting

### Technical Program

**Organized by**

The Chinese Society for Metals (CSM)

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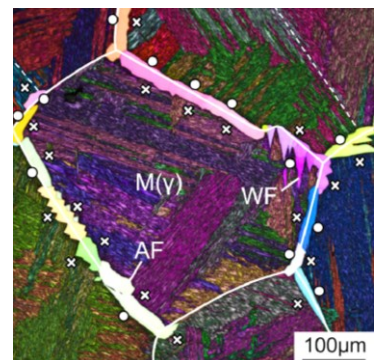
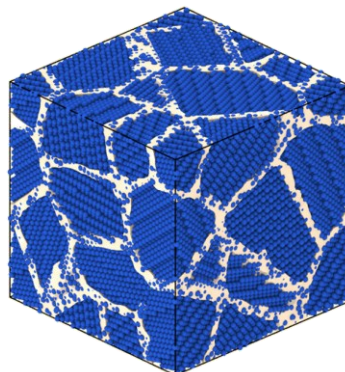
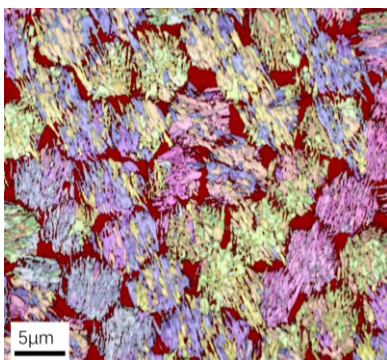
The Japan Institute of Metals and Materials (JIM)

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Conference Website: [www.ptm2020.com](http://www.ptm2020.com)

# The 8th International Conference on Solid→Solid Phase Transformations in Inorganic Materials

June 27<sup>th</sup>- 30<sup>th</sup>, 2022 Virtual Meeting

## Technical Program

*Monday | 27 JUNE 2022 | Day 1 GMT+8 (Beijing)*

### Plenary Session | Zoom Room A

16:00-16:15

Opening Address

16:15-17:15

Tadashi Furuhashi: Interface in solid-solid phase transformation - interplay of kinetics and crystallography ([Hillert-Cahn Lecture](#))

17:15-17:30

Break

17:30-18:30

Alexis Deschamps: Kinetics of phase transformations: What do we learn from in-situ studies?

18:30-19:00

Break

Zoom Room A

Zoom Room B

Zoom Room C

Zoom Room D

Ferrite

Transformation Induced Plasticity I

Magnesium Alloys

Theoretical Modeling I

19:30-20:00

Goro Miyamoto\*

Elena Pereloma\*

Jianfeng Nie\*

Tetsuo Mohri\*

20:00-20:15

Clelia Couchet

Xinfu Gu

Chuang Dong\*

20:15-20:30

Hussein Farahani

Mingxin Huang\*

Xuefei Huang

20:30-20:45

Break

Ferrite and Pearlite

Transformation Induced Plasticity II

Titanium Alloys I

Theoretical Modeling II

20:45-21:15

Nobuo Nakada\*

Feng Liu\*

Hamish Fraser\*

Hongbiao Dong\*

21:15-21:30

Julien Teixeira

Cemal Cem Tasan\*

Yufeng Zheng\*

Zhongwu Zhang\*

21:30-21:45

Jiayi Yan

21:45-22:00

Imed-Eddine Benrabah

Zhiping Xiong

Mariana Rodrigues

Peter W. Voorhees\*

22:00-22:15

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Jiangtao Liang

—

\* Invited

Monday | 27 JUNE 2022

# The 8th International Conference on Solid→Solid Phase Transformations in Inorganic Materials

June 27<sup>th</sup>- 30<sup>th</sup>, 2022 Virtual Meeting

## Technical Program

*Tuesday | 28 JUNE 2022 | Day 2 GMT+8 (Beijing)*

### Plenary Session | Zoom Room A

16:00-17:00

Matthias Militzer: Multi-scale modelling of phase transformations  
– Where do we stand?

17:00-17:15

Break

### Aaronson Award Session | Zoom Room A

17:15-17:30

Alisson Kwiatkowski da Silva

17:30-17:45

Yuxiang Wu

17:45-18:00

Huan Zhao

18:00-18:15

Zongbiao Dai

18:15-18:30

Haokai Dong

18:30-19:00

Break

Zoom Room A

Zoom Room B

Zoom Room C

Zoom Room D

Bainite

Austenite  
Reversion

Aluminium Alloys I

Theoretical  
Modeling III

19:30-20:00

Annika  
Borgenstam\*

Heung Nam Han\*

Yanjun Li\*

Ingo Steinbach\*

20:00-20:15

Shun Tanaka

Haiwen Luo\*

Laure Bourgeois\*

Ernst  
Gamsjaeger\*

20:15-20:30

Zhinan Yang

Xianguang Zhang

Zezhong Zhang

Manon Bonvalet  
Rolland\*

20:30-20:45

Guhui Gao

Break\*\*

Bainite and  
Martensite I

Additive  
Manufacturing I

Aluminium  
Alloys II

Phase Field  
Modelling I

21:00-21:15

Francisca G.  
Caballero\*

Amy Clarke\*

Knut Marthinsen\*

—

21:15-21:30

dos Santos Avila  
Daniel

Eric Lass\*

Benjamin Milkereit

Alphonse Finel\*

21:30-21:45

Arthur Nishikawa

Seiichiro Ii

Farnaz Aghebati

22:00-22:15

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Ayush Suhane

\* Invited \*\*Zoom Room D takes a break at 21:00

Tuesday | 28 JUNE 2022

# The 8th International Conference on Solid→Solid Phase Transformations in Inorganic Materials

June 27<sup>th</sup>- 30<sup>th</sup>, 2022 Virtual Meeting

## Technical Program

*Wednesday | 29 JUNE 2022 | Day 3 GMT+8 (Beijing)*

### Plenary Session | Zoom Room A

16:00-17:00	Christopher Hutchinson: Chemical patterning of alloys			
17:00-17:15	Break			
	Zoom Room A	Zoom Room B	Zoom Room C	Zoom Room D
	Bainite and Martensite II	Additive Manufacturing II	Titanium Alloys II	Phase Field Modelling II
17:15-17:45	Yongchang Liu*	Pedro Rivera-Diaz-del-Castillo*	Tong Li*	Benoit Appolaire*
17:45-18:00	Steve Gaudetz	Yingjie Yao	Renlong Xin	Yann Le Bouar*
18:00-18:15	Alfonso Navarro-Lopez	Hossein Eskandari Sabzi	Zhangzhi Shi	
18:15-19:15	Break			
	Martensite	Additive Manufacturing III	Interfaces	Phase Field Modelling III
19:15-19:45	Wei Xu*	Sophie Primig*	Jianghua Chen*	Katsuyo Thornton*
19:45-20:00	Zhuohui Zeng	Dong Qiu*	James Howe*	Rongpei Shi*
20:00-20:15	Thomas Kohne			
20:15-20:30	Duanjun Sun	Moukrane Dehmas	Jian Luo*	Ryuichiro Oguma
20:30-20:45	Lingyu Wang	—		—
20:45-21:00	Break			
Plenary Session   Zoom Room A				
21:00-21:30	Longqing Chen: A pair of new developments of phase-field method for solid-state phase transformations			

\* Invited

Wednesday | 29 JUNE 2022

# The 8th International Conference on Solid→Solid Phase Transformations in Inorganic Materials

June 27<sup>th</sup>- 30<sup>th</sup>, 2022 Virtual Meeting

## Technical Program

*Thursday | 30 JUNE 2022 | Day 4 GMT+8 (Beijing)*

Thursday | 30 JUNE 2022

Plenary Session   Zoom Room A				
16:00-17:00	Wenzheng Zhang: Role of interfaces on the morphology of phase transformation products			
17:00-17:15	Break			
	Zoom Room A	Zoom Room B	Zoom Room C	Zoom Room D
	Precipitation in Steels	Advanced high strength Steels	High-entropy Alloy and Ni-superalloy	Atomistic Simulation I
17:15-17:30	Sven Erik Offerman	Hongliang Yi*	Zengbao Jiao*	Joerg Neugebauer*
17:30-17:45	Wei Wang			
17:45-18:00	Yongjie Zhang	Qingquan Lai	Weihong Liu	Tilman Hickel*
18:00-18:15	Zhenqiang Wang	Zhangwei Wang	Ziyong Hou	
18:15-19:15	Break			
	Precipitation in Steels	Advanced high strength Steels	Shape Memory Alloy	Atomistic Simulation II
19:15-19:30	Tao Zhou	Yu Zhang	Fei Xiao*	Ying Chen*
19:30-19:45	Javad Mola	Qinyi Guo		Chris Wolverton*
19:45-20:00	Andre Tschiptschin	Ran Ding	Junyu Chen	
20:00-20:15	Qing Chen	Yu Li	Kai Yan	Jinyu Zhang
20:15-20:30	Break			
	Interdiscipline I	Industrial applications	Interdiscipline II	Atomistic Simulation III
20:30-20:45	Eugen Rabkin*	Hélio Goldenstein*	Fulin Jiang	Xiaoqin Ou
20:45-21:00			Santhana Eswara	Pascal Bellon*
21:00-21:15	Andreas Leineweber	Qingyun Sha	Tianyu Ma	
Closing Remarks   Zoom Room A				
21:15-21:30	PTM2022 awards ceremony and closing remarks			

\* Invited



# TECHNICAL PROGRAM

Monday | 27 JUNE 2022 GMT+8 (Beijing)

**Zoom link: TBD**  
**Chairs: TBD**

## 16:00 Opening Address

### 16:15 Plenary (Hillert-Cahn Lecture) Interface in Solid-Solid Phase Transformation - Interplay of Kinetics and Crystallography

*Tadashi Furuhashi<sup>1</sup>; YongJie Zhang<sup>1</sup>; Mitsutaka Sato<sup>1</sup>;  
 Goro Miyamoto<sup>1</sup>; <sup>1</sup>Tohoku University*

Roles of interface crystallography in nucleation and growth of solid-solid phase transformations are introduced. Further, alloy partitioning and precipitation during interphase boundary migration in low-alloy steels are discussed in particular coherency of migrating ferrite/austenite interphase boundary in conjunction with strengthening effects.

## 17:15 Break

### 17:30 Plenary Kinetics of Phase Transformations: What do We Learn from In-Situ Studies?

*Alexis Deschamps<sup>1</sup>; Alexis Deschamps<sup>1</sup>; <sup>1</sup>Université  
 Grenoble Alpes*

This contribution proposes to show how the access to in-situ characterization of phase transformation kinetics has profoundly changed our understanding of their dynamics, and how the access to this kinetics data helps validating and developing predictive models for phase transformations. The in-situ methods that will be presented will be presented, with emphasis on X-rays: small-angle X-ray scattering for nanoscale precipitate characterization, and high energy X-ray diffraction for large fraction phase fraction characterization. Examples will first be given on precipitation kinetics, ranging from simple isothermal heat

treatments to more complex situations: non-stoichiometry, non-sphericity, non-isothermal heat treatments. Then examples will be given on phase transformations in steels, describing the phase fractions and austenite carbon content during early stages of transformation, and the martensitic transformation during plastic deformation of metastable austenite. Finally, we will present our combinatorial approach to map the phase transformation kinetics in compositional space, using compositionally graded alloys in combination with time- and space-resolved X-ray experiments.

## 18:30 Break

### Zoom Room A

## Ferrite

**Zoom link: TBD**  
**Chairs: TBD**

### 19:30 Invited Interaction of Alloying Element with Migrating Ferrite/Austenite Interface

*Goro Miyamoto<sup>1</sup>; Tadashi Furuhashi<sup>1</sup>; <sup>1</sup>Tohoku University*

Phase transformations among austenite, ferrite, pearlite, bainite and martensite are the source of diversity in steel microstructure and various types of steels are developed by microstructure control using phase transformation. One of the key issue in microstructure control by phase transformation is quantitative understanding of interaction of alloying elements with moving interface, which is related to solute drag (hardenability), element partitioning at the interface (TRIP, QP steels), and interphase precipitation (nano-sized carbide strengthening steels). We have investigated interaction of alloying elements with interface quantitatively based on nanoscale enrichment of alloying

element (3DAP), energy dissipation evaluated from interfacial carbon content (FE-EPMA), interfacial orientation relationship (EBSD / reconstruction method). In the presentation, interaction of Mo and Mn with ferrite or bainite / austenite interface will be discussed. Especially, effects of interfacial coherency on segregation behavior of alloying elements will be emphasized because Mo and Mn segregation is suppressed at interface having near K-S orientation relationship compared with non K-S interface although energy dissipation at near K-S and non K-S interfaces are similar. Those measurements will be compared with steady-state and non-steady state solute drag models.

**20:00 Contributed**  
**Ferrite Recovery and Recrystallization Investigated by In Situ High Energy X-Ray Diffraction Experiments**

*Clelia Couchet<sup>1,2</sup>; Sebastien Allain<sup>1</sup>; Julien Teixeira<sup>1</sup>; Marc Moreno<sup>1</sup>; Guillaume Geandier<sup>1</sup>; Frederic Bonnet<sup>2</sup>; <sup>1</sup>Institut Jean Lamour; <sup>2</sup>ArcelorMittal*

Competitive recovery and recrystallization of a conventional low carbon ferritic steel have been investigated in situ thanks to High Energy X-Ray Diffraction experiments and original automated spot tracking methods. These experiments has been carried out on P07 beamline in PETRA III at DESY (Hambourg) with a monochromatic beam (100 keV). High flux from synchrotron source goes through the sample and fast high-throughout 2D detector (Perkin-Elmer) collects Debye-Scherrer (DS) diffraction patterns at significant rate (10 Hz). Four isothermal annealing temperatures (450°C, 500°C, 550°C and 650°C) have been studied. Recovery kinetics has been determined using a modified Williamson-Hall method inspired by Ungar et al. (Appl. Phys. Lett. 69, 3173 (1996)) and compared to the prediction of recovery models. Recrystallization has been followed by tracking isolated diffraction spots on DS rings produced by newly recrystallized grains. This work aims to provide better understanding for recovery and recrystallization processes, both influencing the microstructure morphogenesis and the final mechanical properties of steels.

**20:15 Contributed**  
**A Conditional Local Equilibrium Model of**

**Alloying Effects on Migrating Interfaces**

*Hussein Farahani<sup>1</sup>; <sup>1</sup>Principal Researcher*

The models of solid-state phase transformation with moving interfaces typically consider local equilibrium imposed only for selected alloying elements, usually just interstitial C. This study introduces a new model with some 3 or more elements in which local equilibrium is taken only as the extreme condition satisfied at the interface as a function of interface velocity and diffusion coefficient of each element inside the interface. Such a combination of conditions provides a unique critical interface velocity for each element at each temperature, above which no partitioning of that element occurs across the interface. The interface velocity is calculated by balancing Gibbs energies around the moving interface. The dissipation of energy for the diffusion of every alloying element inside and across the interface is calculated separately with respect to their local interfacial concentrations and considered in balancing Gibbs energies around the interface. Subsequently, the distributions of the alloying elements are updated from their initial profiles, progresses of the interface, and the concentrations at the interface. This new model enables a detailed analysis of the partitioning behavior of alloying elements and their effect on the interface velocity during the entire transformation without a constraining thermodynamic condition. The model is applied to capture the segregation behavior of elements in a series of high strength steels. The results are compared to available experimental measurements and the metallurgical insights are discussed.

**20:30 Break**

**Ferrite and Pearlite**

**Chairs: TBD**

**20:45 Invited**  
**Effect of Internal Stress Accommodation on Plastic Deformation Behavior in Pearlitic Steel**

*Nobuo Nakada<sup>1</sup>; Yutaro Amemiya<sup>1</sup>; Naoki Miyazawa<sup>1</sup>; Makoto Kosaka<sup>2</sup>; Masaharu Kato<sup>2</sup>; <sup>1</sup>Tokyo Institute of*

*Technology; <sup>2</sup>Nippon Steel Corporation*

Accommodation mechanism of internal stress originated from the lattice misfit between ferrite and cementite phases and its effect on plastic deformation behavior were investigated in pearlitic steel. The local analysis of change in the lattice parameter ratio of cementite,  $b/a$  and  $c/a$ , by means of EBSD method reveals that the internal stress in pearlite is dynamically accommodated by two different processes; one is introductions of misfit dislocations and structural ledges on ferrite/cementite lamellar interfaces upon pearlitic transformation (built-in accommodation) and the other is interfacial diffusion of iron atoms (time-dependent relaxation) during annealing after the completion of pearlitic transformation. On the other hand, molecular dynamics simulation demonstrated that the change in internal stress in pearlite by the introduction of misfit dislocations has large influence on the activation of dislocation source in pearlitic ferrite matrix. These results suggest that mechanical properties of pearlitic steels are affected by not only fine lamellar structure but also the internal stress state.

**21:15 Contributed****Refinement of Microstructures after Nitrogen Enrichment and Austenite Decomposition in A Low-alloyed Steel Studied by EBSD and Laser Confocal Scanning Microscopy**

*Julien Teixeira<sup>1</sup>; Madhumanti Mandal<sup>1,2</sup>; Lionel Germain<sup>1</sup>; Florimonde Lebel<sup>1</sup>; Sabine Denis<sup>1</sup>; Nathalie Gey<sup>1</sup>; <sup>1</sup>Université de Lorraine; <sup>2</sup>Institut de Recherche Technologique Matériaux*

Case-hardening treatments, such as carbonitriding are widely used in gear applications. Previous studies showed that nitrogen enrichment of austenite induces strong acceleration of austenite decomposition kinetics and finer resulting microstructures. In order to understand further these effects, present study exploits the possibilities offered by orientation-based microscopy (EBSD) and in situ laser confocal scanning microscopy (LCSM). EBSD analysis supports a previous interpretation: nitrides precipitates formed in austenite during enrichment promote the nucleation of ferrite upon cooling. After re-austenitization followed by water quench, bainite and martensite are preponderant in microstructure, but numerous proeutectoid ferrite grains nucleated on CrN nitrides, both at inter- and

intragranular sites. New outcome from EBSD and LCSM is to show a drastic refinement of the austenite grains upon re-austenitization, which is ascribed in part to the interaction of nitrides with austenite grains upon heating. This finer austenite structure also contributes to faster austenite decomposition and finer resulting microstructures.

**21:30 Contributed****Pearlite in Multicomponent Steels: Phenomenological Steady-state Modeling**

*Jiayi Yan<sup>1</sup>; John Ågren<sup>1</sup>; Johan Jeppsson<sup>1</sup>; <sup>1</sup>Thermo-Calc Software AB*

A steady-state model for austenite-to-pearlite transformation in multicomponent steel is presented, including Fe, C, and eight more elements. The model considers classic ingredients but also finite austenite-pearlite interfacial mobility which resolves some previous difficulties. A transition between orthopearlite and parapearlite is realized by optimizing the partitioning of substitutional alloying elements under constrained carbon equilibrium between ferrite and cementite. Solute drag effect is included to account for the bay in growth rate curves, which also affects lamellar spacing and partition coefficient. Grain boundary nucleation rate is modeled as a function of chemical composition, driving force, and temperature, with consideration of grain boundary equilibrium segregation. Overall transformation kinetics is obtained from growth rate and grain boundary nucleation rate, assuming pearlite colonies only nucleate on austenite grain boundaries. Further theoretical and experimental work are suggested for generalization and improvements, including a better understanding of the non-Arrhenius temperature dependence of austenite-pearlite interfacial mobility by ledge mechanism.

**21:45 Contributed****Use of Space-resolved In-situ high Energy X-ray Diffraction for the Characterization of the Compositional Dependence of the Austenite-to-ferrite Transformation Kinetics in Steels**

*Imed-Eddine BENRABAH <sup>1</sup>; Hugo Paul VAN LANDEGHEM <sup>1</sup>; Frédéric BONNET <sup>2</sup>; Guillaume GEANDIER<sup>3</sup>; Benoit DENAND<sup>3</sup>; and Alexis DESCHAMPS<sup>1</sup>; <sup>1</sup> Université Grenoble Alpes; <sup>2</sup> Research,*



*ArcelorMittal, Maizières-les-Metz ; <sup>3</sup> Université de Lorraine*

A combinatorial methodology to study the effect of substitutional elements on ferrite growth kinetics in Fe-C-X and Fe-C-X-Y systems is presented in this study. It involves the fabrication of materials with macroscopic composition gradients, and their characterization by *in situ* high-energy X-Ray diffraction (HEXRD). One ternary system (Fe-C-Ni) has been selected to illustrate the applicability of the combinatorial approach in studying such transformations.

### Zoom Room B

## Transformation Induced Plasticity I

**Zoom link:** TBD

**Chairs:** TBD

### 19:30 Invited

#### On the Stability of Retained Austenite in Transformation-Induced Plasticity Steels

*Elena Pereloma<sup>1</sup>; Zhiping Xiong<sup>1,2</sup>; Ahmed Saleh<sup>1</sup>; Azdiar Gazder<sup>1</sup>; Jiangting Wang<sup>3</sup>; Ross Marceau<sup>3</sup>; Ilana Timokhina<sup>3</sup>; <sup>1</sup>University of Wollongong; <sup>2</sup>Beijing Institute of Technology; <sup>3</sup>Deakin University*

The morphology and carbon content in retained austenite (RA) in Transformation-Induced Plasticity (TRIP) steel was characterised using correlative electron backscattering diffraction, transmission electron microscopy and atom probe tomography. The response of RA to applied load was evaluated using nanoindentation. The long-term room temperature stability of retained austenite in thermo-mechanically processed TRIP steel was also investigated. The results showed that carbon concentration in RA does not depend on its morphology (film-like or blocky) but on the neighbouring phases. The high inhomogeneity of carbon within and between the RA grains affects their both mechanical and chemical stability. Different RA grains could undergo either deformation-induced martensite

transformation or twinning, or both, in the same steel. The decomposition of a significant fraction of RA into pearlite was observed after 16 years storage at room temperature.

### 20:00 Invited

#### Abnormal TRIP Effect on Strain Hardening Behavior of Steel at High Strain Rate

*Mingxin Huang<sup>1</sup>; Ming Wang<sup>1</sup>; <sup>1</sup>The University of Hong Kong*

The transformation of metastable austenite to martensite, which is referred to transformation-induced plasticity (TRIP) effect, generally results in an enhancement of strain hardening rate of TRIP-assisted steels. Nevertheless, the present work observes an abnormal TRIP effect in a Quenching and partitioning (Q&P) steel. Although a considerable amount of retained austenite transformed to martensite during the tensile test at a strain rate of 1000 s<sup>-1</sup>, no obvious enhancement of strain hardening rate was observed. To explore the underlying mechanisms for such an abnormal TRIP effect, the evolution of dislocation density and martensitic transformation were characterized by synchrotron X-ray diffraction and electron microscopy. Comparing the quasi-static and high-strain-rate results, it is found that the dislocation density in the martensite matrix is suppressed at 1000 s<sup>-1</sup>, resulting in a lower strain hardening rate. Furthermore, the transformed martensite deforms plastically at 1000 s<sup>-1</sup>. Without the composite-like deformation behaviour (elastically in hard transformed martensite and plastically in soft martensite matrix), the corresponding strain hardening rate is reduced.

### 20:30 Break

## Transformation Induced Plasticity II

**Chairs:** TBD

### 20:45 Invited

#### Metallic materials design by generalized stability

*Jingbin Zhang<sup>1</sup>; Feng Liu<sup>1</sup>; Haiwen Luo<sup>2</sup>; <sup>1</sup>Northwestern Polytechnical University; <sup>2</sup>University of*

*Science & Technology Beijing*

Designing structured materials with optimized mechanical properties generally focuses on engineering microstructures, which are closely determined by the processing routes, such as phase transformations (PTs) and plastic deformations (PDs). Both PTs and PDs follow inherent trade-off relation between thermodynamic driving force  $\Delta G$  and kinetic energy barrier  $Q$ , i.e., so-called thermo-kinetic correlation. By analyzing nucleation and growth and proposing a conception of negative driving force integrating strain energy, interface energy and any kind of energy that equivalently inhibits the PT itself,  $\Delta G$ s, unified expressions for the thermo-kinetic correlation and generalized stability (GS) were derived for three kinds of PTs, i.e., diffusive PTs with simultaneously decreased  $\Delta G$  and increased  $Q$ , diffusive PTs with simultaneously increased  $\Delta G$  and decreased  $Q$ , and displacive PTs with simultaneously increased  $\Delta G$  and decreased  $Q$ . This leads to so-called thermo-kinetic connectivity by integrating the thermo-kinetic correlation and the GS, where, by application in typical PTs, it was clearly shown, a criterion of high  $\Delta G$ -high GS can be predicted by modulating chemical driving force, negative driving force and kinetic energy barrier for diffusion or nucleation. Following thermo-kinetic connectivity, analogous procedure for dislocation evolution upon PDs was performed. It was verified the high  $\Delta G$ -high GS concept against a phase transformation-modulated nanostructured Fe alloy, for which an ultrahigh yield strength of 2.61 GPa and an ultimate compressive strength of 3.32 GPa while having a total strain to failure of 35% are achieved via multiple strengthening and hardening mechanisms. The materials design in terms of the high  $\Delta G$ -high GS criterion was discussed to assist in the rapid selection of phase transformations to facilitate superior mechanical properties, finally.

**20:45 Invited****Ferrite effects in the mechanically-induced martensitic transformation in QP steels**

*Jiyun Kang<sup>1</sup>; Cem Tasan<sup>1</sup>; <sup>1</sup>MIT*

Understanding factors governing strain localization and damage in QP steels is challenging, due to the complexity of the microstructure with multiple constituents. In this

investigation, we combine in-situ SEM and in-situ synchrotron diffraction experiments to shed more light on neighbourhood effects. More specifically, we clarify the role of ferrite in the mechanically-induced martensitic transformation of the metastable austenite.

**21:45 Contributed****Effect of retained austenite on fracture behaviors of third-generation advanced high-strength steels**

*Zhiping Xiong<sup>1</sup>; <sup>1</sup>Beijing Institute of Technology*

A systematic investigation on the evolution of fracture resistance with microstructure is essential and necessary for advanced high-strength steels; whereas, the focus is often put on the strength-ductility tradeoff. This presentation deliberately deals with the dependence of fracture resistance on the morphology and distribution of martensite/retained austenite (RA/M) constituent in a Fe -0.3 C - 2.5 Mn - 1.5 Si - 0.8 Cr (wt. %) steel processed by quenching & partitioning (Q & P) and isothermal bainite transformation (IBT). Tensile properties and fracture resistance are characterized using uniaxial tension and double edge-notched tension. For Q & P process, with decreasing quenching temperature, the amount of blocky RA decreases while the amount of film RA comparatively increases, leading to an increase in fracture resistance. For IBT process, with increasing IBT temperature, the fracture resistance decreases due to an increase in the size of blocky RA/M island and a decrease in the interspace between these islands. A coarse size of and a small interspace between block RA/M islands are detrimental to the fracture resistance due to the promotion of crack nucleation and crack propagation, respectively. It is emphasized here that tensile properties are mainly affected by the stability and amount of RA while the fracture resistance is also affected by the size and distribution of blocky RA/M islands. For enhancing the balance between tensile properties and fracture resistance, a control of the amount and morphology of RA/M should be considered in order to simultaneously keep large tensile ductility and to avoid easy crack nucleation and propagation.

**22:00 Contributed****Effect of Retained Austenite Morphology on the Hydrogen Induced Cracking Behavior of Transformation Induced Plasticity Steel**

*Jiangtao Liang<sup>1,2</sup>; Kun Liu<sup>1,2</sup>; Hui Pan<sup>1,2</sup>; Fei Li<sup>1,2</sup>; Zhihong Tian<sup>1,2</sup>; Feifan Xu<sup>1,2</sup>; Yajun Hui<sup>1,2</sup>; Ronghua Cao<sup>1,2</sup>; <sup>1</sup>Shougang Research Institute of Technology; <sup>2</sup>Beijing Key Laboratory of Green Recyclable Process for Iron & Steel Production*

In this study, two kinds of transformation induced plasticity (TRIP) steels with different retained austenite morphology (equiaxed retained austenite and lamellar retained austenite) were designed. The transformation behavior of equiaxed retained austenite and lamellar retained austenite under hydrogen charging was compared. The transformation of retained austenite is more rapid after hydrogen charging, almost all retained austenite transforms at low strain. The steel with lamellar retained austenite shows lower strength loss (Sloss) and elongation loss (Eloss) after slow strain rate test (SSRT). Compared with the equiaxed retained austenite, the lamellar retained austenite exhibits better hydrogen embrittlement resistance. On the one hand, the lamellar retained austenite shows the continuous TRIP effect during stretching, which improves the formability and energy absorption performance during collision. On the other hand, the lamellar retained austenite decreases the sensitivity of the hydrogen embrittlement and ensures the safety of the parts. This result can guide the microstructure design of the third generation ultra strong automotive sheet.

*<sup>2</sup>Chongqing University*

Precipitation hardenable aluminium and magnesium alloys are two important groups of engineering light alloys. Mechanical properties of these alloys depend critically on their microstructures which are strongly influenced by alloying elements and heat treatment processes. In conventional transmission electron microscopy, whilst information on the identity, spatial distribution and chemistry of precipitates could be readily obtained, it was difficult to reveal, at the atomic scale, the distribution of solute atoms or atoms of micro-alloying elements. It was for this reason that the roles of micro-alloying elements in precipitation of key strengthening intermetallic phases remained unresolved. Advances in scanning transmission electron microscopy (STEM) in the past 15 years, especially the aberration-corrected STEM techniques including high-angle annular dark-field (HAADF) and energy-dispersive X-ray spectroscopy (EDS), provide opportunities for detecting segregated solute atoms at the atomic scale. The purpose of this talk is to provide a review of the progress made in the understanding of precipitation and the role of micro-alloying elements in precipitation in selected aluminum and magnesium alloys, highlighting the importance of modern imaging and spectroscopy techniques of STEM in the characterization and development of these light alloys.

**Zoom Room C**

**Magnesium Alloys**

**Zoom link: TBD**  
**Chairs: TBD**

**20:00 Invited**  
**Characterization of Solute Segregation and Precipitates in Light Alloys Using Advanced Scanning Transmission Electron Microscopy Techniques**

*Jian-Feng Nie<sup>1</sup>; Houwen Chen<sup>2</sup>; <sup>1</sup>Monash University;*

**20:00 Contributed**  
**The Effect of Grain Boundary on Precipitation Crystallography in Magnesium Alloy**

*Xinfu Gu<sup>1</sup>; Ping Yang<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing*

Precipitation on deformation defects is essential for enhancing mechanical properties of age-hardenable alloys. The deformation defects act as heterogeneous nucleation sites and promote precipitation; in turn, these precipitates pin the movement of effects and improve the mechanical properties. Similar to other alloy systems, the precipitates in magnesium alloy also often exhibit preferred crystallographic features, such as specific orientation relationship (OR) between precipitates and matrix, interfacial orientation, morphology, and growth direction. These crystallographic features are one of the determinant

factors of mechanical properties. Therefore, the understanding of precipitation crystallography at deformation defects in magnesium is indispensable in controlling the mechanical properties, but the related studies are limited. The crystallographic restriction of deformation defects on precipitation was studied in the alloy systems mostly with cubic matrix due to the importance of steel, titanium alloy, etc. In magnesium alloys, twinning is an important deformation mode to accommodate the deformation strains due to limited slip systems. Therefore, it is important to study the effect of the twin boundary (TB) on the precipitation process.

In this work, we revealed how TB influences precipitation in Mg-Al-Zn alloys. As-cast Mg-9Al-1Zn (AZ91) alloy was homogenized at 415 °C for 24 hours and subsequently quenched by water. Compression samples with outer diameter of 10 mm and height of 15 mm were cut from the solution-heat-treated sample and then compressed at room temperature with ~ 4 pct strain to introduce the proper amount of deformation twins. Finally, the samples were aged at 300 °C for 2 to 6 hours. The method for preparing TEM specimens was prepared by ion milling. The TEM observation was carried out with Talos F200 (200 kV, FEI, OR, USA), and the statistic study of the crystal orientation was based on EBSD (Oxford Instruments, Oxfordshire, England).

It is shown that the precipitates on the TBs are different from those in matrix. Most precipitates hold the reproducible OR only with twin or matrix. Moreover, certain precipitate variants are absent and a new rule for variant selection on TB is proposed. In addition, the precipitation behavior on TB is compared with these at general grain boundaries.

### 20:15 Contributed

#### Characterization and Interpretation on the Multiple Crystallographic Features of the $\epsilon'$ Precipitates in an Mg-Sn-Ag-Zn-Mn Alloy

*Xuefei Huang<sup>1</sup>; Wenzheng Zhang<sup>2</sup>; Weigang Huang<sup>1</sup>; <sup>1</sup> Sichuan University; <sup>2</sup> Tsinghua University*

The  $\epsilon'$ -Mg<sub>54</sub>Ag<sub>17</sub> precipitates play an important role in the age-hardening response of the Mg-Sn-Ag-Zn-Mn alloy. This work reported the multiple crystallographic features (i.e., orientation relationship with respect to the matrix, interface

orientations) of the  $\epsilon'$ ; precipitates. The orientation relationships of the two main types of the precipitates look much similar, but definitely different. The reason why these interface orientations appeared were consistently explained by the secondary constrained coincidence site lattice (II-CCSL) model. Namely, they are preferred due to their smaller interface misfit. The detailed microscopic interfacial structures (such as structural ledges or rational flat planes) of the facets were calculated by the model, and they are in good agreement with the HRTEM observations. A comprehensive evaluation on the interface misfit and the lattice strain to sustain the II-CCSL structure showed that either type of the precipitates is clearly superior than the other one. Moreover, a growth-ledge-aided morphology evolution path of one type of the precipitates was proposed according to the experimental results, indicating that both thermodynamic and kinetic factors should be considered on understanding the precipitates morphology.

### 20:30 Break

## Titanium Alloys

Chairs: TBD

### 20:45 Invited

#### The Influence of Nano-scale Structural Instabilities on Microstructural Evolution in Metastable Beta Titanium Alloys

*Hamish Fraser<sup>1</sup>; Yufeng Zheng<sup>2</sup>; Dong Wang<sup>3</sup>; Rajarshi Banerjee<sup>4</sup>; Dipankar Banerjee<sup>5</sup>; Yunzhi Wang<sup>1</sup>; <sup>1</sup>The Ohio State University; <sup>2</sup>University of Nevada Reno; <sup>3</sup>Xi'an Jiaotong University; <sup>4</sup>University of North Texas; <sup>5</sup>Indian Institute of Science*

A variety of nano-scale structural instabilities formed in different metastable  $\beta$  titanium alloys have been systematically investigated using advanced characterization techniques. The characteristics of three different types of nano-scale structural instabilities, the transformation mechanisms and pathways involved and the critical experimental conditions to generate such nano-scale phases



will be reviewed and summarized, including athermal  $\omega$  phase with hexagonal structure, O'; phase with orthorhombic structure, and incommensurate modulated nanodomains. The athermal  $\omega$  phase has been observed in the as-quenched state in Ti-xMo (x=12, 15 and 18), Ti-18Mo-5Al, Ti-20V, Ti-5Fe, Ti-5Al-5Mo-5V-3Cr (Ti-5553) and Ti-24Nb-4Zr-8Sn (Ti-2448), compositions in wt.% unless otherwise specified. O' phase has been characterized to co-exist with athermal  $\omega$  phase in the as-quenched state isomorphous titanium alloys, including Ti-26Zr-2Al (at.%), Ti-18Mo, Ti-18Mo-5Al, Ti-5553 and Ti-2448. Incommensurate modulated nanodomains were found in compositionally graded Ti-xFe alloy when the athermal  $\omega$  phase is suppressed. The influence of these various nano-scale structural instabilities on microstructural evolution, particularly the formation of dispersions of refined distributions of the alpha phase, has been determined. Thus, the omega phase may have direct and indirect influences, and in the absence of this phase, it has been determined that the pseudo-spinodal transformation mechanism can be activated. These various transformation pathways will be discussed. The support of the US National Science Foundation, Metals and Metallic Nanostructures, Division of Materials Research, is gratefully acknowledged.

### 21:15 Invited

#### O' Phase: An Example of Shuffle Transformation in the Metastable Beta Titanium Alloys

*Yufeng Zheng<sup>1</sup>; Dong Wang<sup>2</sup>; Yunzhi Wang<sup>3</sup>; Rajarshi Banerjee<sup>4</sup>; Dipankar Banerjee<sup>5</sup>; Hamish Fraser<sup>3</sup>; <sup>1</sup>University of Nevada Reno; <sup>2</sup>Xi'an Jiaotong University; <sup>3</sup>The Ohio State University; <sup>4</sup>University of North Texas; <sup>5</sup>Indian Institute of Science*

Shuffle transformation is a distinct class of displacive transformation, accomplished by the rearrangement of atom positions within the unit cell, with little or no pure strain of the lattice. For example, the beta to athermal omega phase transformation in the metastable beta titanium alloy is a prototype shuffle transformation. During cooling from bcc beta phase solid solution, the hexagonal structured athermal omega phase is formed by the shuffle of every two of three adjacent {111} planes in the bcc lattice towards the intermediate plane of the two,

leaving the third plane unaltered. Recently, a novel shuffle transformation, beta to O' phase transformation, has been explored in the metastable beta titanium alloy for the first time using advanced electron microscopy. In this work, the mechanism of beta to O' phase transformation and the influence the solute concentration and temperature on the O' phase will be introduced. The characterization using aberration-corrected scanning transmission electron microscopy in Ti-18Mo, Ti-18Mo-5Al, Ti-5Al-5Mo-5V-3Cr and Ti-24Nb-4Zr-8Sn (wt%) has clearly shown that the nano-scaled O' phase of the orthorhombic structure transforms from beta phase by the shuffle of every other {110} planes of bcc lattice along the <1-10> directions. O' phase cannot be suppressed by quenching, as long as the solute concentration of the metastable beta titanium alloy exceeds a critical value. O' phase has been observed to be stable from room temperature to the elevated temperature up to the O' phase solvus temperature, via in-situ heating transmission electron microscopy.

### 21:45 Contributed

#### In-situ Laser Ultrasonic Measurements of Molybdenum Effects on Phase Transformation Kinetics in Ti-Mo Alloys

*Mariana Rodrigues<sup>1</sup>; Matthias Militzer<sup>1</sup>; Mariana Rodrigues<sup>1</sup>; <sup>1</sup>The University of British Columbia*

The growth of the aerospace industry during the last couple decades has driven increasing employment of  $\beta$  titanium alloys as structural materials in aircraft components. These alloys are attractive for aerospace application as they have high yield strength and good fatigue and crack propagation properties in addition to their inherent low specific density and outstanding corrosion resistance. Among the  $\beta$  stabilizing elements, molybdenum is one of the most commonly used in commercial titanium alloys. In comparison with other traditional  $\beta$  stabilizers, such as vanadium and chromium, molybdenum possesses the lowest diffusion rate in the  $\beta$  phase and, therefore, determines the  $\alpha/\beta$  phase transformation rates. While most of earlier studies focused on complex multicomponent Ti-systems, here we investigate binary Ti-Mo model alloys with systematically varied Mo content up to 6 wt.% to elucidate in detail the effect of Mo on the phase transformation kinetics. A Gleeble

thermomechanical simulator coupled with a Laser Ultrasonics for Metallurgy (LUMet) sensor was used to measure the phase transformation rates in these Ti-Mo alloys during continuous heat treatments. In this technique, the measurably different densities and elastic constants of the parent and product phases result in variation in the ultrasound longitudinal velocity, which is related to the transformed volume fractions. The results show a significant reduction in transformation kinetics with increasing molybdenum content that can be correlated to the rejection rates of Mo from the  $\alpha$  phase. Based on the experimental observations a phenomenological transformation model is being proposed that accounts for the kinetic role of Mo. This study is encouraging for a wider use of the laser ultrasonics technique as a real time, non-contact and non-destructive tool for microstructural evolution investigations during complex thermomechanical processes in industrial Ti-alloys.

## Zoom Room D

### Theoretical Modeling I

**Zoom link:** TBD

**Chairs:** TBD

**19:30 Invited**

#### Theoretical Study of Atomic Size and Phase Transformation

*Tetsuo Mohri<sup>1</sup>; Tetsuo Mohri<sup>1</sup>; <sup>1</sup>Tohoku University*

It is well known that a system with a large difference in atomic size of constituent elements becomes unstable in a disordered solid solution, leading to a phase transformation. Although the atomic size of a constituent element in an alloy has been a central subject for the alloy theory, not much theoretical studies have been advanced particularly for a concentrated solid solution. This is partly due to the fact that a local lattice distortion which is closely related to an atomic size is not readily separated from the total atomic displacement. Additional difficulty arises in estimating

entropy effects at finite temperatures originating from the atomic distributions of displaced atoms around a Bravais lattice point. By combining Kanzaki force, which was reformulated by Khachatryan, with Cluster Variation Method and Continuous Displacement Cluster Variation Method, we attempted to calculate atomic sizes of Cu and Au in a Cu-Au solid solution. In fact, thermodynamic properties of Cu-Au system have been well studied both theoretically and experimentally. Yet, calculated thermodynamic quantities and properties such as heats of mixing and phase diagram have much room for improvement. The discrepancies have been attributed to the neglect of accurate estimation of the local lattice distortion. In the present study, we developed Continuous Displacement Cluster Variation Method (CDCVM) which is the natural extension of the Cluster Variation Method to continuous space. It has been confirmed that CDCVM with Lennard-Jones system provides significantly improved topology of a phase diagram. Also, the Gaussian-shaped atomic distribution around a Bravais lattice point is confirmed. The internal energy is estimated from the first-principles calculations through Cluster Expansion Method operated on a set of total energies of selected ordered compounds including L12 and L10 phases. In the conventional CVM calculations, we minimize the free energy with respect to cluster probabilities, equivalently correlation functions, and a volume of the system, leading to a global lattice relaxation. For the present study, we minimize the free energy directly with respect to atomic size of Cu and Au under a given temperature and chemical potential. By changing the chemical potential, concentration dependences of the heats of formation and atomic size in a solid solution are calculated at 720K at which experimental results are available. As compared with the global lattice relaxation for which heats of formation is underestimated, indicating that the disordered phase is under-stabilized, the present results provide closer agreement with experimental results. It is interesting that atomic size of both the constituent elements in a solid solution maintain the size in the pure state of each element. The physical significance of the present results are discussed based on Eshelby cycle and Kanzaki force in both real- and k-space formulation.

**20:00 Invited**

**Cluster-Based Structural Model and Composition Genes for Materials**

*Chuang Dong<sup>1,2</sup>; Shuang Zhang<sup>1</sup>; Cunlei Zou<sup>1</sup>; Chenxi Dong<sup>1</sup>; Yajun Zhao<sup>1</sup>; <sup>1</sup>Dalian Jiaotong University; <sup>2</sup>Dalian University of Technology*

High-performance materials always possess specific chemical compositions, which strongly suggest the possible existence of some molecule-like structural units, in which the versatile but specific compositions are rooted. These structural units mimic the molecules in chemical substances but generally differ from the crystallographic unit cells. The possibility of having these fundamental units has been apparently overlooked because of the lack of structural models to properly address the short-range order in materials. Our research group has already proposed the cluster-plus-glue-atom model in 2007, which is a short-range-order structural model that renders any structure with a structural unit containing the essential structural information of the whole system. From the nomination of this model, one immediately determines a molecule-like structural unit consisting of a nearest-neighbor cluster plus a few outer-shell glue atoms. Actually, such structural unit, serving as the composition carrier, can be seen as the composition gene of the material. In the present work, Friedel oscillations, in combination with the cluster-plus-glue-atom model, are fully presented to show how to uncover the composition genes hidden in chemical short-range orders in any material. Examples are given in three categories of materials, i.e., metallic alloys including solid solutions and metallic glasses, inorganic compounds as well as relevant glasses, and polymers. Furthermore, materials can be classified into single-, dual-, and multi-gene types. The proposition of composition genes facilitates the understanding of prevailing materials and can be a useful tool to guide the exploration of new composition space.

**20:30 Break**

**Theoretical Modeling II**

**Chairs: TBD**

**20:45 Invited**

**Data-driven Modelling of BOF Steelmaking**

*Hongbiao Dong<sup>1,2</sup>; Xingzhong Liang<sup>1</sup>; <sup>1</sup>University of Leicester; <sup>2</sup>Tsinghua University*

**21:15 Invited**

**Phase Transformation via Atomic-scale Periodic Interfacial Energy**

*Ye Cui<sup>1</sup>; Yang Zhang<sup>1</sup>; Lixin Sun<sup>1</sup>; Mikhail Feygenson<sup>2</sup>; Mingyu Fan<sup>1</sup>; Xun-Li Wang<sup>3</sup>; Peter K. Liaw<sup>4</sup>; Ian Baker<sup>5</sup>; Zhongwu Zhang<sup>1</sup>; <sup>1</sup>Harbin Engineering University; <sup>2</sup>Jülich Centre for Neutron Science (JCNS-1); <sup>3</sup>City University of Hong Kong; <sup>4</sup>The University of Tennessee; <sup>5</sup>Dartmouth College*

Displacive and diffusional transformations are the main processes during solid-state phase transformations, which have formed the basis of applied physics and materials technology for centuries. However, the relationship between diffusional and displacive transformations has remained elusive, which significantly hinders the fundamental understanding and control of the microstructures and properties of materials via phase transformations. Here, we introduce the concept of a periodic differential interfacial energy between atom layers. We develop the mechanism of an atomic-scale displacive process in the form of atoms groups (cells) based on the periodic differential interfacial energy and experimentally determine the displacive short-range order (SRO) cell size in an Mg-Li alloy using a neutron total scattering method. We proposed that the origins of both the displacive and diffusional transformations are displacive in nature governed by the driving force of transformations. Our work paves the way for building a bridge correlating the nature of various solid-state phase transformations.

**21:45 Invited**

### **Interface Migration and Pinning in Stressed Solids**

*Nicholas J. Weadock<sup>3</sup>; Brent Fultz<sup>2</sup>; Peter W. Voorhees<sup>1</sup>;  
<sup>1</sup>Northwestern University; <sup>2</sup>California Institute of  
Technology; <sup>3</sup>SLAC National Accelerator Laboratory;*

A possible route to storing hydrogen for hydrogen-based energy systems is via hydride formation. One challenge of using metal hydrides to store hydrogen is an efficiency loss due to hysteresis: the absorption and desorption of hydrogen does not occur at the same hydrogen gas pressure. We examine phase formation, phase equilibria, and interfacial migration in the hydrogen-palladium system where a significant difference in lattice parameters between the hydride and matrix phases generates stress in the system. The stress is thought to lead to a coherent phase equilibrium state that induces the hysteresis. However, experiment shows that the hysteresis is present even in a partially transformed system, indicating that a stress-induced jump in volume fraction of hydride is not responsible for the hysteresis. An explanation for the hysteresis is given that is based upon the driving force for interface migration that results from the superstition of hydrogen and the stress that is generated by the mismatch between phases, and interface pinning due to dislocations and other lattice defects.



Tuesday | 28 JUNE 2022 GMT+8 (Beijing)

Zoom link: TBD

Chairs: TBD

### 16:00 Plenary

#### Multi-scale Modelling of Phase Transformations – Where do We Stand?

*Matthias Militzer; The University of British Columbia*

With the advances in computational materials science simulations of microstructure evolution and phase transformations have been carried out in the past two decades across different length and time scales. In particular, multi-scale modelling has been promoted in the framework of Integrated Computational Materials Engineering (ICME). Here, it is sought to combine atomistic scale simulations with meso-scale modelling on the microstructure length scale to eventually develop predictive tools for the industrially relevant macro-scale. The present lecture will provide a critical assessment of the achievements and limitations of this approach with an emphasis on phase transformation in advanced high-performance low carbon steels. The discussion will in particular focus on the effect of alloying elements on the phase transformation kinetics. The challenges of coarse graining atomistic scale simulations will be analyzed. Phase field modelling will be presented as the meso-scale simulation methodology of choice for microstructures with complex morphologies, e.g. bainitic and Widmanst&auml;ml; tten ferrite, as frequently observed in advanced steels. Based on a number of case studies, a general outlook will be given on future directions of phase transformation modelling.

### 17:15 Break

#### Aaronson Awards Session

### 17:15

#### Interplay of Segregation and Spinodal Phenomena and their Relevance to Heterogeneous Nucleation

*Alisson Kwiatkowski da Silva<sup>1</sup>; Dirk Ponge<sup>1</sup>; Baptiste Gault<sup>1</sup>; Dierk Raabe<sup>1</sup>; <sup>1</sup>Max-Planck-Institut für Eisenforschung GmbH*

Nucleation remains the less well understood step in the complete thermodynamic sequence that shapes a microstructure. Nucleation is usually described using the classical nucleation theory (CNT). CNT describes the formation of the nucleus of the new phase from solution in a single step by stochastic fluctuations and the preferential nucleation (heterogeneous nucleation) of a phase at internal defects, such as grain boundaries and dislocations, is usually attributed only to the reduction in interfacial energy. Nevertheless, nucleation often proceeds via multiple steps and spinodal decomposition is a common pathway for nucleation (e.g. via formation of GP zones in some Al-alloys). Additionally, solid state segregation to internal defects is known to locally alter the driving force for phase transition by changing the chemical composition of the interfacial region. In this overview, I will give a summary of recent progress we proposed in the understanding of the thermodynamics and kinetics of grain boundary segregation, confined spinodal phenomena and its interplay with heterogeneous nucleation. I will cover (i) the characterization of solute segregation to internal defects in the bulk, and first order transitions in adsorption; (ii) the thermodynamics and kinetics of solute segregation; and (iii) the interplay of solute segregation and nucleation. I will cover examples in multiple alloy systems, with an emphasis on the Mn segregation and austenite reversion in martensitic Fe-Mn alloys, given the industrial relevance of this system.

### 17:30

#### Cementite Coarsening during the Tempering of Multicomponent Martensite

*Yuxiang Wu<sup>1</sup>; Wenwen Sun<sup>1</sup>; Xiang Gao<sup>1</sup>; Mark Styles<sup>2</sup>; Artem Arlazarov<sup>3</sup>; Christopher Hutchinson<sup>1</sup>; <sup>1</sup> Monash University; <sup>2</sup> CSIRO Manufacturing; <sup>3</sup> ArcelorMittal Global Research and Development*

During the solid-state precipitation in multicomponent systems, the difference in the diffusivities of different species in precipitate or matrix could lead to a time-

dependent evolution of precipitate/matrix chemistry. This has been reported in a number of engineering alloys and in steel metallurgy where C and substitutionals have orders of magnitude differences in diffusivities, the stoichiometric cementite phase, (Fe, M)<sub>3</sub>C, precipitates with the evolution of partitioned substitutional composition of M during the tempering of multicomponent martensite.

Martensite tempering has a direct technological importance related to current extensive development of advanced high strength steels (AHSS). It is often included as an intermediate annealing process between hot-rolling and cold-rolling stages and leads to Mn-partitioned cementite. This will be the starting microstructure for austenite formation during intercritical annealing and the Mn-partitioned cementite is known to have a strong influence on the austenite formation kinetics. The aim of this contribution is to provide a better understanding of cementite precipitation kinetics during martensite tempering and can then benefit the processing optimisation of AHSS.

In this work, both the cementite chemistry and particle size evolution have been quantitatively monitored experimentally during the tempering of multicomponent martensite at temperatures between 400°C and 600°C. Cementite precipitation in alloyed steels, such as Fe-C-Mn, is a coarsening reaction (with decreasing particle number density) that occurs under conditions where the Mn content of the cementite is continually evolving (increasing significantly during coarsening). In this respect, it is not a pure coarsening problem where the evolution is driven only by capillarity, and the pure coarsening process in multicomponent systems has been described by Björklund, Donaghey and Hillert (1972), Morral and Purdy (1994), and Kuehmann and Voorhees (1996). In the time frame of this transient coarsening, the carbon diffusion is driven by capillarity, but the Mn redistribution and partitioning are driven by composition gradients in the martensite matrix. In this work, we present a new model that can simultaneously describe both the evolution of the cementite particle size and chemistry during coarsening. In this model, we employ a coupled two-particle setup and each particle characterises the dissolving and growing fraction of the size distribution of precipitates under coarsening respectively. Diffusion both within the matrix and within the cementite is described, and

the different driving forces for the C and Mn fluxes that determine the operative tie-lines at the particle/matrix interface are respected. We have first simulated and compared with the experimentally measured Mn partitioning kinetics and growth kinetics over a range of compositions and temperatures in the Fe-C-Mn ternary systems. The uncertainty of substitutional diffusion in cementite is highlighted. Based on this framework, we further generalise the model to higher-order systems containing both anti-segregating elements (Si and Al) and segregating elements (Mn, Cr and Mo) to cementite and their effects on cementite size and chemistry evolution are discussed.

**17:45**

### **Defect induced phase transformation and hydrogen embrittlement in high-strength Al alloys**

*Huan Zhao<sup>1</sup>; Poulami Chakraborty<sup>1</sup>; Liam Huber<sup>1</sup>; Wenjun Lu<sup>1</sup>; Tilmann Hickel<sup>1</sup>; Binhan Sun<sup>1</sup>; Dirk Ponge<sup>1</sup>; Baptiste Gault<sup>1</sup>; Dierk Raabe<sup>1</sup>; <sup>1</sup>Max-Planck-Institut für Eisenforschung*

Interplay of chemistry and structure at grain boundaries and their impact on the phase transformation during aging was investigated at near-atomic-scale in a high-strength 7xxx Al alloy. It shows that the solute segregation during aging accelerates the precipitation sequence at grain boundaries compared to bulk and the self-consistent coevolution of facet structure and chemistry is observed at grain boundaries. Near-atomic-scale analysis of hydrogen shows that hydrogen is trapped in second-phase particles and at grain boundaries. Atomistic ab initio calculations show that the co-segregation of alloying elements and hydrogen favours grain boundary decohesion, and the strong partitioning of hydrogen into the second-phase particles removes solute hydrogen from the matrix, hence preventing hydrogen embrittlement.

**18:00**

### **Mechanism of Phase Transformation and Metastable Austenite Tailoring in Fe-C-Mn-Si Q&P Steels**

*Zongbiao Dai<sup>1</sup>; Chi Zhang<sup>1</sup>; Zhigang Yang<sup>1</sup>; hao Chen<sup>1</sup>; <sup>1</sup>Tsinghua University*

Metastable austenite in the quenching and partitioning (Q&P) steels is mainly obtained through carbon partitioning from martensite into austenite during partitioning. However, carbon partitioning is usually accompanied with complex competitive reactions, e.g. formation of Cottrell atmospheres and carbides in martensite (i.e. incomplete carbon partitioning (ICP) phenomenon), Mn partitioning across the martensite/austenite interface, martensite/austenite interface migration or bainite formation. A so-called incomplete carbon partitioning-local equilibrium (ICP-LE) model, in which the martensite/austenite interface is assumed to be in local equilibrium condition, is proposed to clarify the interactions between the various metallurgical phenomena during the Q&P process. The current model is capable of predicting the evolution of austenite fraction and its carbon content during partitioning in the Fe-C-Mn-Si steels.

**18:15**  
**On the Role of Nb Interface Segregation in Ferrite Transformation of Low Carbon Steels**

*Haokai Dong<sup>1</sup>; Yongjie Zhang<sup>2</sup>; Goro Miyamoto<sup>2</sup>; Hao Chen<sup>3</sup>; Zhigang Yang<sup>3</sup>; Masahiro Inomoto<sup>4</sup>; Tadashi Furuhashi<sup>2</sup>; <sup>1</sup>South China University of Technology; <sup>2</sup>Tohoku University; <sup>3</sup>Tsinghua University; <sup>4</sup>Kobe Steel, Ltd.*

Nb addition strongly delays ferrite transformation kinetics by suppressing both ferrite nucleation and growth. The origin of growth retardation has been recognized to be caused by solute drag effect (SDE) through Nb segregation at the  $\alpha/\gamma$  interface. However, the relations between Nb segregation, SDE and interface velocity have not been clarified yet. Occurrence of NbC interphase precipitation during ferrite growth may also change segregation behavior of Nb whereas the resultant effect remains unclear. Therefore, in the present work, Fe-0.1C and Fe-0.1C-(0.03, 0.06)Nb (mass%) alloys subjected to the isothermal heat treatments at 750oC-825oC have been used to study the role of Nb interface segregation on ferrite transformation. The amount of Nb segregation, energy dissipation at the interface, and interface velocity have been experimentally determined. Three-dimensional atom probe confirms that Nb can segregate at the migrating interface without any orientation relationship but is absent at the K-S interface. Amount of Nb

segregation at the non K-S interface increases with longer reaction time, while energy dissipation estimated from the interfacial C content decreases with time and increases with decreasing transformation temperatures. The SDE model with optimized segregation parameters can reproduce the relations between amount of Nb segregation, energy dissipation and interface velocity. NbC interphase precipitation affects the transformation rate indirectly by weakening the SDE via consumption of Nb solutes in ferrite. In contrast, their pinning effect plays a marginal role.

**18:30 Break**

**Zoom Room A**

**Bainite**

**Zoom link: TBD**  
**Chairs: TBD**

**19:30 Invited**  
**A Morphological Study of Bainite**

*Annika Borgenstam<sup>1</sup>; <sup>1</sup>KTH Royal Institute of Technology*  
 A systematic survey of the morphology of bainite as well as proeutectoid ferrite in Fe-C alloys will here be presented. It will be shown that there is a gradual change in morphology with decreasing temperature between Widmanstätten ferrite and the ferritic component of upper bainite, as well as between upper and lower bainite in contradiction to previously presented observations of a sharp transition between the two. The reason to this difference is due to the definition the distinction is based on and will here be discussed. Bainite forms through a combination of lengthening, thickening and widening. The first two have been studied extensively and are fairly well understood while widening seems to have been much neglected but some aspects will here be highlighted. Other observations to be discussed are the stages for formation of upper bainite; the formation of parallel plates of ferrite and the

transformation of the interspaces to a mixture of cementite and ferrite.

#### 20:00 Contributed

##### The Carbon Enrichment in the Retained Austenite with Bainite Transformation for Fe-0.1%C-0.5%Si-2.0%Mn Alloy

*Shun Tanaka<sup>1</sup>; Hiroyuki Shirahata<sup>1</sup>; Genichi Shigesato<sup>1</sup>; <sup>1</sup>Nippon Steel Corporation*

Bainitic ferrite transformation kinetics and carbon enrichment of the retained austenite during isothermal holding at 500 — 600°C for Fe - 0.1mass%C - 0.5mass%Si - 2.0mass%Mn alloy was investigated. The transformation rapidly progressed until about 50 s and then stasis was observed (1st stage). The carbon concentration of the retained austenite was measured by FE-EPMA. The carbon concentration increased as the transformation proceeded and showed almost constant value during the stasis. It reached to about 0.45 — 0.50% at 550°C, which is the T' composition with 100 J/mol of additional energy. After the stasis, a slight increase of the ferrite or bainitic ferrite fraction was detected by the dilatometry (2nd stage). The carbon concentration of the retained austenite also increased and reached to about 0.60%, which clearly exceeded the T composition and was close to the WBs composition or the limit of NPLE prediction. It is considered that at the first stage bainite transformation occurred and showed the incomplete transformation, and then at the second stage diffusional ferrite transformation proceeded with NPLE mode. These results imply that the incomplete bainite transformation was determined by the T' composition and the stasis of the following ferrite transformation was provided by the limit of NPLE mode. However, as Wu (2017) discussed, it is necessary to consider the possibility that the transformation is predicted in the overall temperature range by the WBs limit theory which gives the additional dissipation energy from the para-equilibrium.

#### 20:15 Contributed

##### A Discussion on the Effect of Preformed Martensite on Bainite Transformation

*Zhinan Yang<sup>1</sup>; <sup>1</sup>Yanshan University*

Shortening the bainite transformation time is one crucial issue on the application of bainite steel, especially of high

carbon nano-bainite steel. Many methods have been studied to accelerate bainite transformation, and introducing a certain amount of martensite before bainite transformation have been demonstrated to be effective on shortening the transformation time. However, we recently found that the martensite effect did not work at low temperature, which presented a shortened incubation time and an unchanged whole transformation time. For the same steel transformed at a relatively higher temperature, the acceleration effect works. The phase transformation kinetic is analyzed and the mechanism of martensite effect is discussed in this paper. And two kinds of steel, high carbon and medium carbon, were also introduced and the effect of martensite on the two steels were compared. There is no doubt that the incubation time is notably shortened due to the reduced activation energy barrier for nucleation at the phase boundary of martensite/austenite. The further transformation process is influenced by the grain size and the stability of untransformed austenite. We hope to reveal the real effect mechanism of martensite on the bainite transformation through this study.

#### 20:30 Contributed

##### Effect of Chemical Microsegregation on the Transformation Behavior and Wear Resistance of Bainitic Rail Steel for Heavy Haul Railway

*Guhui Gao<sup>1</sup>; Chunlei Zheng<sup>2</sup>; Xiaolu Gui<sup>1</sup>; Zhunli Tan<sup>1</sup>; Bingzhe Bai<sup>1</sup>; Yuqing Weng<sup>1</sup>; <sup>1</sup>Beijing Jiaotong University; <sup>2</sup>Yanshan University*

The heavy haul railway is the most effective way to improve the freight capacity, which is also the development direction of China Railway. With increased axle load, traffic capacity and density, the heavy haul railway requires that the rail steels have more excellent strength, toughness, fatigue and wear resistance. Compared with conventional pearlite rail steels, the bainitic rail steels have higher strength, toughness and RCF resistance, and hence have been attracted many attentions in the past two decades. The alloying design is important to obtain desirable bainitic microstructure in rail steels. In this case, the alloying microsegregation produced during casting process is usually inevitable and cannot be eliminated completely by means of heat treatment. Any change in chemical composition must influence the



transformation thermodynamics and kinetics and hence affect mechanical properties. In this paper, we discussed the effect of microsegregation on the transformation behavior and wear resistance of bainitic rail steel via laboratory and field tests. The microstructural characterizations revealed that the banded structure was formed along rolling direction due to the chemical segregation in the bainitic rail steel. The microstructures of positive-segregation area and negative segregation area are mainly martensite and bainite, respectively. Meanwhile, the banded structure exhibits a nonuniformly distribution microhardness. The twin disc wear test in Lab revealed that an increase in degree of segregation enabled material to improve the wear resistance through the improvement of local hardness of the rail, but seriously reduced the rolling contact fatigue performance of the rail. The in-fielding test showed that the banded structure promoted the multilayer White and Brown Etching Layer (WEL and BEL) heterostructure on the surface/subsurface of worn bainitic rail. It is suggested that the heterogeneous microstructure and chemical micro-segregation in parent material induced the localized grain refinement, oxidation, and embrittlement under plastic deformation and temperature rise upon wheel-rail contact, which was responsible for the formation of multilayer WEL/BEL heterostructure in bainitic rail steels. Based on the results, the new chemical and microstructure design concepts were proposed to improve the resistance of both wear and rolling contact fatigue of bainitic rail steels.

**20:45 Break**

### Bainite and Martensite I

Chairs: TBD

**21:00 Invited**

### Examining the Multi-scale Complexity of Isothermally Treated Bainitic and Martensitic Structures

*Francisca G. Caballero<sup>1</sup>; David De-Castro<sup>1</sup>; Rosalia*

*Rementeria<sup>1,2</sup>; Thomas Sourmail<sup>3</sup>; Jonathan D. Poplawsky<sup>4</sup>; Esteban Urones-Garrote<sup>5</sup>; Jose Antonio Jimenez<sup>1</sup>; Carlos Capdevila<sup>1</sup>; <sup>1</sup>National Center for Metallurgical Research (CENIM-CSIC); <sup>2</sup>ArcelorMittal Global R&D; <sup>3</sup>Asco Industries Research (CREAS); <sup>4</sup>Center for Nanophase Materials Sciences (ORNL); <sup>5</sup>Spanish National Centre for Electron Microscopy (CNME)*

Bainitic and martensitic structures with similar hardness can be obtained by adjusting the isothermal holding temperature of austempering, quench and partitioning (Q&P) and quench and tempering (Q&T) at low temperatures (230°C). In this work, resultant ferritic structures are compared using multiple characterisation techniques including X-ray diffraction, electron back scatter diffraction, scanning and transmission electron microscopy, and atom probe tomography. Results revealed that austenite content is the same for the three treatments conditions; as well as structural characteristics such as the tetragonality in ferrite, microstrain and crystallite size of the structure measured by XRD. Only nano-scale examination of the precipitation state allows differentiation of bainite and martensite treated at low temperatures. On the other hand, electron back scatter diffraction investigation revealed the crystallographic ferritic grains in the bainitic structure to be coarser than those in Q&P and Q&T martensitic structures treated at the same temperature. The larger driving force related to martensitic transformation in Q&P and Q&T structures is thought to be responsible for the detected crystallographic refinement, fundamental for improving fracture toughness and fatigue performance of materials.

**21:30 Contributed**

### Modeling the Effect of Grain Size on Bainite Formation Kinetics

*Daniel dos Santos Avila dos Santos Avila<sup>1</sup>; S Erik Offerman<sup>2</sup>; Maria J Santofimia<sup>2</sup>; <sup>1</sup>TU Delft; <sup>2</sup>Delft University of Technology*

The influence of the austenite grain size on bainite formation kinetics has raised controversy in the literature. Experiments have shown that grain refinement accelerates bainite formation in some steels but slows it down in others. The most accepted theory is that this influence is governed by the

difference in the rate of grain boundary and autocatalytic bainite nucleation. To investigate the topic, we modified a model for diffusionless bainite formation, limiting the fraction of bainite nucleated at grain boundaries and at the bainite/austenite interfaces by considering the length of the bainitic sub-unit and the austenite grain size. The modified model was able to fit well data from the literature for bainite formation kinetics of a steel with varying grain sizes, and it accurately captured the increased importance of autocatalysis for coarser grains. The model also indicated that increasing grain size decreases the activation energy for bainite formation, possibly by softening the austenite matrix.

### 21:45 Contributed

#### Modeling Bainite Reaction Using a Cellular Automata Model

*Arthur Nishikawa<sup>1</sup>; Kees Bos<sup>1,2</sup>; Maria J. Santofimia<sup>1</sup>; Arthur Nishikawa; <sup>1</sup> TU Delft; <sup>2</sup> Tata Steel Europe*

Cellular automata (CA) models represent a low computational cost alternative for modeling phase transformations, being able to describe the polycrystalline morphology of phases, providing information of grain sizes and composition gradients. A cellular automaton consists of a grid in which each cell has a set of states/properties, such as composition and nature of the phase; the evolution of a CA system is defined by a set of rules describing how the neighboring cells interact to each other modifying their respective states. In 2010, Bos et al. (2010) developed a 3D CA model able to describe the relevant phase transformations occurring during the annealing of dual phase steels. This is achieved by multiple submodels implemented in the CA framework, such as for describing the austenite formation from ferrite and pearlite, recrystallization of ferrite, and the decomposition of austenite to pro-eutectoid ferrite. In this model, currently known as Cellular Automata Phase Transformation Sharp Interface (CASIPT), cells of a given phase that are neighboring cells of a different phase are called interface cells. The growth of a phase is described by capture rules applied to these special interface cells. This model represents a valuable tool for the microstructural prediction of dual phase steels, but cannot be applied to the formation of bainite. This represents a strong limitation for

the application of the model, since bainite plays an important role on the design of advanced high-strength steels. The present work describes the ongoing development of a 3D cellular automata model describing the bainite transformation from austenite as a submodel in the CASIPT framework. Growth of bainite occurs with bainitic ferrite establishing specific orientation relationships and habit planes with respect to the parent austenite grain, developing lath or plate-like morphologies. This mechanism contrasts with the isotropic growth of polygonal ferrite, currently implemented in the CASIPT model. Such different mechanisms imply that the growth rules used for ferrite growth cannot be used for describing bainite growth. For tackling this problem, a new "unidirectional off-centered" capture rule has been developed by assuming that the thickening and widening rates of bainite are negligible when compared to its lengthening rate. In order to establish a compromise between the level of detail of the phenomena of interest and the computational cost of the simulations, in the model the ferrite and carbide phases are not represented individually and bainite is assumed to be a pseudo-phase instead. For further simplification, a bainite "grain" is assumed to be a group of bainite laths with similar orientations. Crystallographic orientations are taken into account in the model and the orientation relationship of bainite (bainitic ferrite) with respect to austenite is assumed to be Kurdjumov-Sachs. The kinetics of precipitation of carbides inside the bainite pseudo-phase is described by a set of analytical equations. The rate of the carbides precipitation determines the fraction of carbon rejected to austenite, which in turn is used to calculate the velocity of the austenite/bainite interface by means of the mixed-model approach. Since thickening and widening of bainite are neglected, the shape of a bainite grain is strongly affected by the shape of the initial bainite nucleus. Results show that the model is able to reproduce realistic bainitic microstructures. By changing the dimensions of the nuclei, different bainite morphologies corresponding to different transformation temperatures are obtained. Good agreement between the predicted and experimental overall kinetics of transformation was obtained. It is proposed that similar growth rules can be applied for modeling other

transformations involving the growth of lath or plate-like products, such as the martensite transformation.

## Zoom Room B

### Austenite Reversion

Zoom link: TBD

Chairs: TBD

#### 19:30 Invited Microstructure Resetting of Metastable Austenitic Alloys Based on Electroplasticity Concept

*Heung Nam Han<sup>1</sup>; Hye-Jin Jeong<sup>1</sup>; Moon-Jo Kim<sup>2</sup>; Ju-Won Park<sup>1</sup>; Howook Choi<sup>1</sup>; Viet Tien Luu<sup>3</sup>; Sung-Tae Hong<sup>3</sup>; <sup>1</sup>Seoul National University; <sup>2</sup>Korean institute of industrial technology; <sup>3</sup>University of Ulsan*

The microscale defects in materials act to damage the originally designed microstructure during their use, which degrades their mechanical properties/life expectancy. Therefore, various methods for healing or repairing the damage in materials have been proposed based on self-healing concept. Among them, we utilized a subsecond electric pulsing to reset the damaged microstructure of metastable austenitic alloys as a non-autonomous self-healing method. It is known that the kinetic of microstructural changes such as dislocation annihilation, aging, dissolution, and recrystallization was accelerated due to athermal effect as well as Joule heating, when a high density of electric pulsing is applied to metallic materials. The microstructure reset assisted infinite deformation was realized in 301L stainless steel by the selection of resetting cores as the reverse transformation from strain-induced martensite to austenite and the recrystallization of deformed austenite. For NiTi alloy, the reverse transformation of remained stress-induced martensite to austenite was chosen as a main resetting core with dislocation recovery. It was confirmed that the damaged structure after over 100 cyclic

tests were successfully returned to the initial state through the subsecond electric pulsing.

#### 20:00 Invited Substantial Strengthening Mechanism of Medium Mn Steel During Ultrafast Heating: Martensitic, Massive or Bainitic Reverse Transformation?

*Pengyu Wen<sup>1</sup>; Haiwen Luo<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing*

Ultrafast heating (UFH) at the rates of 10-300 °C/s was employed to anneal cold-rolled 7wt% Mn steel sheets. In comparison to the conventional long intercritical annealing, the UFH processes produced larger fraction of RA grains (up to 37%) containing high density of dislocations, leading to the significant increase in yield strength by 270 MPa and the product of strength and elongation up to 55 GPa% due to the enormous work hardening capacity. The results on the microstructural characterization, thermodynamics calculation on the reverse transformation temperature and the kinetic simulations all suggest that the austenitization during UFH is displacive and involves the diffusion and partition of C. Therefore, we propose that it is a bainite-like transformation.

#### 20:30 Contributed A Comparative Study of Austenite Reversion Behavior from Martensitic and Bainitic Initial Structures

*Xianguang Zhang<sup>1</sup>; Goro Miyamoto<sup>2</sup>; Lifeng Zhang<sup>1</sup>; Tadashi Furuhashi<sup>2</sup>; <sup>1</sup>University of Science and Technology Beijing; <sup>2</sup>Tohoku University*

Microstructure evolution during austenite reversion from martensitic or bainitic structures is of great important for production of TRIP steel. Two morphologies of austenite, i.e., acicular and globular, are known to form during reversion from lath martensite or bainite. It was reported that initial microstructure, such as fresh and tempered martensite and bainite, influences kinetics and morphologies of austenite reversion. However, the effects of initial microstructure on austenite reversion in Fe-Mn-Si-C alloy have not been investigated systematically yet. In this study, we aim to investigate the austenite reversion from various initial structures to reveal effects of cementite distribution and its

compositions and presence of retained austenite. It was found that globular austenite formation at high temperature is enhanced in the initial structures of pre-tempered martensite and BF+ cementite which have larger cementite particles, while it is suppressed by presence of retained austenite. Larger cementite particles show a strong nucleation potency which may promote the formation of globular austenite.

**20:45 Break**

## Additive Manufacturing I

**Chairs: TBD**

### **21:00 Invited** **Microstructure Development under Additive Manufacturing Conditions**

*Amy Clarke<sup>1</sup>; <sup>1</sup>Colorado School of Mines*

Additive manufacturing (AM) typically produces large temperature gradients, high solidification velocities, and repeated cycles of heating and cooling. A common characteristic of as-printed metallic alloys is the growth of coarse columnar grains that may impact mechanical response, so ways to control microstructure evolution are of great technological interest. Combinations of thermal gradient (G) and solid/liquid interface velocity (V) are known to significantly impact microstructure development, including potential grain refinement produced by the columnar to equiaxed transition (CET). Thus, a deeper understanding of solidification (and solid state phase transformations, when appropriate) under AM conditions is needed to guide the design of alloys matched to AM processes. State-of-the-art, multiscale characterization of solidification dynamics and resulting microstructures in the context of the local conditions experienced during AM is needed to achieve this aim. Here we highlight new insights into microstructure development under AM conditions obtained by in-situ/ex-situ characterization of conventional alloys, model alloys, and alloys designed for AM. These results will inform solidification modeling and enable the

prediction and control of microstructure evolution under AM conditions.

### **21:30 Invited** **Phase Transformations and Microstructural Evolution During Post-Build Thermal Processing of Additively Manufactured Alloys**

*Eric Lass<sup>1</sup>; <sup>1</sup>The University of Tennessee*

Additive manufacturing (AM) has received significant attention in recent years because of its potential to transform the commercial production of components, particularly for high-value, low-volume applications, where part geometries and other requirements make them difficult or impossible to produce via conventional processing methods. One inherent drawback to current AM technology is the reproducibility of microstructures and properties of materials created via the additive process. This is because most of the alloys currently in use for AM applications were originally developed for dramatically different processing routes, namely conventional cast and/or wrought processes. Thus, the microstructures and properties of alloys built using AM processes can be dramatically different than nominally identical wrought counterparts. In many cases, properties also show significant variation from build to build using the same AM process, making component design using such materials impossible. In the present work, we investigate the processing-structure-relationships in additively manufactured materials, focusing on thermal processing in the solid state, i.e. post-built material. Specifically, Inconel 625 and 17-4 PH stainless steel are investigated. As expected, as-built microstructures are comparable to welded materials, and they respond in a similar manner to thermal processing as welded alloys. However, differences are also observed, resulting from the unique processing history of AM alloys compared to conventional materials. For example, composition differences arising from the gas atomization of powder feedstock. Using both computational modeling and experimental investigation the differences in microstructural evolution behavior of conventional and AM materials are highlighted; and post-build thermal processing regimens are identified to develop more uniform predictable AM-produced microstructures. Finally, the future of AM will also be discussed, where the dream is to employ alloys



specifically designed to take advantage of AM processing instead of repurposing alloys designed for other applications. Some possible considerations for AM alloy design will be discussed.

## Zoom Room C

### Aluminium Alloys I

Zoom link: TBD

Chairs: TBD

#### 19:30 Invited

#### Electric Current Induced Abnormal Nucleation and Grain Growth Behavior during Recrystallization of Deformed Aluminium Alloys

*Yanjun Li<sup>1</sup>; Shubo Wang<sup>1</sup>; Hailong Jia<sup>1</sup>; Ragnvald Mathiesen<sup>1</sup>; <sup>1</sup>Norwegian University of Science and Technology*

It is well known that an application of electric current during annealing of cold-deformed metal alloys can accelerate the recrystallization behavior. Although different hypotheses have been proposed, the mechanism behind still remains as a mystery. In this work, a high density electric current heat treatment has been used to anneal cold deformed aluminium alloys. The resulting grain structure and texture have been carefully characterized. More importantly, the nucleation and grain growth kinetics during recrystallization of the alloy under the influence of electric current has been quantitatively studied in-situ by using synchrotron X-ray diffraction approach. Based on the experimental results, a new mechanism is proposed, which can satisfactorily explain the abnormal recrystallization behaviors induced by electric current.

#### 20:00 Invited

#### In situ Transformations of Precipitate Phases in Aluminium Alloys

*Laure Bourgeois<sup>1</sup>; Zezhong Zhang<sup>1,2,3</sup>; Yong Zhang<sup>1</sup>;*

*Julian Rosalie<sup>5</sup>; Yiqiang Chen<sup>1,4</sup>; Nikhil Medhekar<sup>1</sup>; <sup>1</sup>Monash University; <sup>2</sup>University of Antwerp; <sup>3</sup>University of Oxford; <sup>4</sup>Thermofisher Scientific; <sup>5</sup>Erich Schmid Institute of Materials Science*

Many phase transformations associated with solid-state precipitation look structurally simple yet take place with great difficulty. Classic cases of surprisingly difficult phase transformations can be found in alloy systems forming the basis of a broad range of high-strength lightweight aluminium alloys. In these systems, the difficult nucleation of strengthening phases, which are usually semi-coherent, is often preceded by the easy nucleation of another phase with strong structural similarities, typically a coherent precipitate. It is therefore of interest to investigate the reasons behind the difficult transformation from coherent to semi-coherent precipitate phases. Here we examine several phase transformations from pre-existing coherent precipitates in the model alloy systems Al-Cu and Al-Ag, through a combination of atomic resolution scanning transmission electron microscopy and atomistic simulations. We show that certain microalloying additions, or different processing conditions applied to samples in bulk or nanoscale form, result in previously unreported precipitate phases [1-2] or promote the nucleation of existing phases [3-4]. The nucleation mechanisms of these phases involve structural templates provided by coherent precipitates [1-3] and depend critically on the availability of vacancies [1-2,4]. Based on our observations atomic-scale mechanisms are proposed for the coherent to semi-coherent precipitate phase transformation pathways and the associated energy barriers estimated. These findings suggest new approaches to stimulate these phase transformations. References: [1] Z. Zhang, L. Bourgeois, J.M. Rosalie and N.V. Medhekar, *Acta Mater.* 132 (2017) 525. [2] L. Bourgeois, Y. Zhang, Z. Zhang, Y. Chen and N.V. Medhekar, under review. [3] Y. Chen et al. *Acta Mater.* 125 (2017) 340. [4] Y. Zhang, Z. Zhang, N.V. Medhekar and L. Bourgeois, *Acta Mater.* 141 (2017) 341. [5] The authors acknowledge funding from the Australian Research Council, computational support from the Monash Sun Grid cluster, the National Computing Infrastructure and Pawsey Supercomputing Centre funded by the Australian Government, and the use of facilities within the Monash Centre for Electron Microscopy.

**20:30 Contributed****Advanced Imaging and Simulation of Precipitate Interfaces in Aluminium Alloys and their Role in Phase Transformations**

*Ze Zhong Zhang<sup>1,2,3</sup>; Laure Bougeois<sup>3</sup>; Yong Zhang<sup>3</sup>; Julian Rosalie<sup>4</sup>; Nikhil Medhekar<sup>3</sup>; <sup>1</sup>University of Antwerp; <sup>2</sup>University of Oxford; <sup>3</sup>Monash University; <sup>4</sup>Erich Schmid Institute of Materials Science*

Physical metallurgy concerns the fundamentals and applications of phase transformations – the process by which atoms arrange themselves from one structure to another in metallic systems. While pure metals are genuinely soft, metal alloys can be greatly strengthened by precipitation -- the formation of intermetallic phases -- thus enabling the use of alloys in various engineering applications. Once a secondary phase forms within a matrix, heterophase interfaces are generated, and the growth of the precipitate phase is accompanied by the migration of its interfaces. Classical phase transformation theory can rationalise the critical role of interfaces in terms of thermodynamics and kinetics. However, the detailed structures of the precipitate interfaces have rarely been characterised at the atomic scale until recently, revealing complicated but well-defined interfacial structures. This fact is not considered in classical analytical models (e.g. Becker model and Cahn-Hilliard model), which assume the interface to be sharp (an abrupt change from the precipitate phase to the matrix) or diffuse (a concentration gradient from the precipitate phase to the matrix). The associated atomic mechanisms, which underpin phase transformations, remain poorly understood. First-principles methods such as density functional theory (DFT) are often used to address the atomic behaviours. However, the lack of precise experimentally-based interfacial structures prevent accurate atomistic predictions even for the simplest cases. The  $\gamma'$  (Ag<sub>2</sub>Al) phase in the Al-Ag alloy system has served as a textbook example for understanding phase transformations, precipitating hexagonal close-packed (HCP) crystals in the face-centred cubic (FCC) aluminium matrix. The  $\gamma'$  precipitates display fully coherent interfaces at their broad facets and semicoherent interfaces at their edges. Shockley partial dislocations are expected to decorate the semi-coherent interface due to the FCC-HCP structural transformation. Determining the exact locations and core

structures of interfacial dislocations, however, remains challenging. Here we used aberration-corrected scanning transmission electron microscopy and atomistic simulations to re-visit the classical Al-Ag system [1]. We characterised and explained the Ag segregation at coherent interfaces in the early stage of precipitation. For semicoherent interfaces, interfacial dislocations and reconstructions were revealed by bridging advanced microstructure characterisation and atomistic simulations. In particular, we discovered a new FCC/HCP interfacial structure that displays a unique combination of Shockley partial, Lomer-Cottrell and Hirth dislocations that evolve from the known interfacial structure purely composed by Shockley partial dislocations. Our findings show that the FCC-HCP transformation is more complex than hitherto considered, due to the interplay between structure and composition confined at interfaces. Despite its textbook status, the Al-Ag system has not revealed all its phase transformation secrets. For instance, we recently discovered a new phase  $\zeta$  (AgAl) in the binary system [2].

Using this combined approach of advanced imaging and atomistic simulation, we also studied the precipitate-matrix interfaces in various other simple systems, including Al-Cu [3,4], Al-Au [5], Al-Cu-Au [6], Al-Cu-Ag [7] and Al-Cu-In-Sb [8] alloys. Our results demonstrate that DFT calculations can predict reliably the segregation behaviour of solute at precipitate interfaces, at least when the structural configurations of the segregation are known. This corroborates earlier work on the segregation at precipitate interfaces in aluminium and implies that first-principles computations will become increasingly important in the quantitative evaluation of the structural characteristics of precipitate phases when used in concert with atomic-scale experimental characterisation techniques. References:

[1] Zhang, Z., Rosalie, J.M., Medhekar, N.V. and Bougeois, L., *Acta Materialia* 174 (2019): 116-130. [2] Zhang, Z., Bougeois, L., Rosalie, J.M. and Medhekar, N.V., *Acta Materialia* 132 (2017): 525-537. [3] Bougeois, L., Dwyer, C., Weyland, M., Nie, J. F., & Muddle, B. C., *Acta Materialia* 59 (2011): 7043-7050. [4] Bougeois, L., Medhekar, N.V., Smith, A.E., Weyland, M., Nie, J.F. and Dwyer, C. *Physical review letters* 111 (2013): 046102. [5] Bougeois, L., Zhang, Z., Li, J., & Medhekar, N. V., *Acta Materialia* 105 (2016): 284-293. [6] Chen, Y., et al. *Acta Materialia* 125

(2017): 340-350. [7] Rosalie, J. M., Bourgeois, L., & Muddle, B. C. *Acta Materialia* 59 (2011): 7168-7176. [8] Zhang, Y., Zhang, Z., Medhekar, N.V. and Bourgeois, L. *Acta Materialia* 141 (2017): 341-351. [9] The authors acknowledge funding from the Australian Research Council, computational support from the Monash Sun Grid cluster, the National Computing Infrastructure and Pawsey Supercomputing Centre funded by the Australian Government, and the use of facilities within the Monash Centre for Electron Microscopy.

## 20:45 Break

### Aluminium Alloys II

Chairs: TBD

#### 21:00 Invited

#### Particle Effects during Recrystallization of Aluminium Alloys and their Influence on the Texture Evolution

*Knut Marthinsen<sup>1</sup>; Håkon Wiik Ånes<sup>1</sup>; <sup>1</sup> Norwegian University of Science and Technology*

Most commercial aluminum alloys have a complex microchemistry in the form of solid solution levels of alloying elements, volume fraction and size of constituents and dispersoids, and, which may be strongly modified during thermomechanical processing, and which may strongly affect the final recrystallized microstructure and texture. The most significant effects are related to second phase particles, and their influence on both nucleation and growth of recrystallized grains. Large particles will generally promote recrystallization, through the mechanisms of particle stimulated nucleation (PSN), while a high density of small particles (dispersoids) will generally give rise to a significant drag force (Zener pinning), acting on moving sub-grain and grain boundaries (of growing recrystallization grains) and may strongly retard, and in some cases even completely suppress recrystallization. These effects can be particularly strong in conditions of simultaneous

recrystallization and precipitation (i.e. concurrent precipitation) resulting in a sluggish recrystallization reaction, inhomogeneous grain structure of coarse elongated grains and often unconventional textures. However, although extensively studied, the detailed mechanisms by which second-phase particles in general and in particular (concurrent) precipitation affects the nucleation and growth behavior of different texture components are not well understood. The present work will review current knowledge and understanding of the effects of particles on the recrystallization behavior of aluminium alloys and in particular their influence on the texture evolution. Recent results trying to correlate the precipitation behavior of dispersoids and the orientation distribution of nucleation and growth of recrystallization grains (and thus the final texture) will be presented and discussed.

#### 21:30 Contributed

#### In Situ High-Energy X-ray Diffraction of Precipitation and Dissolution Reactions during Heating of Al Alloys

*Hannes Froeck<sup>1</sup>; Christian Rowolt<sup>1</sup>; Benjamin Milkereit<sup>1</sup>; Michael Reich<sup>1</sup>; Wolfgang Kowalski<sup>1</sup>; Andreas Stark<sup>2</sup>; Olaf Kessler<sup>1</sup>; <sup>1</sup>University of Rostock; <sup>2</sup>Institute of Materials Research*

During heating of Al alloys, typically a sequence of precipitation and dissolution reactions occurs and the single (partly opposing) reactions superimpose. Differential scanning calorimetry (DSC) is one common technique to analyse the kinetic development of precipitation and dissolution in Al alloys, but the superposition of the exothermic precipitation and endothermic dissolution reactions complicates the DSC signal interpretation, as DSC measures the sum of any heat effect. Synchrotron high-energy X-ray diffraction (HEXRD) allows the kinetic development of phase transformations to be obtained and can support the separation of superimposed DSC signals. HEXRD results from this work offer a new approach to separate part of the superimposed reactions and their kinetic development for the equilibrium phases beta-Mg<sub>2</sub>Si in EN AW-6082 and eta-Mg (Zn,Cu,Al)<sub>2</sub> in EN AW-7150. Comparing DSC and HEXRD results confirms serious overlap issues. Common DSC evaluation methods alone,

using zero crossing between endothermic and exothermic heat flow or peak positions can be misleading regarding individual reaction start and finish temperatures as well as regarding reaction intensities, which can be unambiguously determined by in situ HEXRD.

### 21:45 Contributed

#### Elastic Strain Evaluation around the Precipitates in Al-Cu Alloys by Transmission Electron Microscopy

*Seiichiro II<sup>1</sup>; Toru HARA<sup>1</sup>; <sup>1</sup>National Institute for Materials Science*

Precipitates in Al alloys play an important role in the improvement of mechanical properties, and it is crucial to control the structure, size, and density of the precipitates and interface between the precipitates and the matrix in Al alloys. On the other hand, remarkable developments of the (scanning) transmission electron microscopy ((S)TEM) have become able to characterize the microstructure with quantitative analysis. Recently, the elastic strain around the precipitates/matrix interfaces in aged Al alloys such as 6XXX and 7XXX has also been quantitatively evaluated. In this study, we characterize the elastic strain around the interface between several kinds of the precipitates and the matrix in aged Al-Cu alloys by Cs-corrected (S)TEM on an atomic scale and the subsequent image analysis. The material used in this study is Al-4.0 mass% Cu alloy plate. Disks with the 3mm in diameter were cut from the plate and solutionized at 823K for 7.2ks. They were aged at 453K for various periods. (S)TEM specimens were prepared by jet polishing and observed by JEOL ARM-300F (Grand ARM) equipped probe and image corrector. The elastic strain around the interface was analyzed by the geometrical analysis and the peak pair analysis techniques. In the Al-4.0 mass% Cu alloy aged for 0.6 ks, we observed the dense GP(I) zones. The elastic strain was clearly exhibited across the precipitates and ununiform in the GP(I) precipitates. Little elastic strain in the matrix around the precipitate can be seen. We also observed GP(II) zones in the specimen aged at the same temperature for 7.2 ks. As for the GP(II) zones, which two Cu layers sandwich a few Al layers, the elastic strain around the precipitates can be also seen and it was much higher than that around the GP(I) precipitates.

### Zoom Room D

#### Theoretical & Data-based Modeling III

Zoom link: TBD

Chairs: TBD

### 19:30 Invited

#### Intelligent-data-guided Process Design for Fatigue-resistant Bainitic Steel:iBain

*Ingo Steinbach<sup>1</sup>; <sup>1</sup>Ruhr University Bochum*

Bainitic steels represent technologically important materials whose fatigue properties are strongly dependent on the microstructure, which in turn is highly sensitive to the manufacturing process. Bainitic microstructures are hierarchically multi-scale and exhibit structural properties down to the nanoscale. Therefore, already the experimental characterization is highly complex and strongly dependent on the subjective experience of the experimenter. Consequently, bainitic steels represent an optimal case study for materials integration, i.e. the combination of experimental research, datadriven approaches and direct microstructure simulation. We combine: A systematic approach to the characterization of microstructures. Reduction of the "human factor". Uncovering unknown relationships beyond the canon of classical metallurgy. Correlation process microstructure material properties – service lifetime. Creating the conditions for intelligent data-driven process design. A short-term added value for the industry is the automated workflow management system, which will be applicable to own material process systems even without in-depth expert knowledge, thus adding significant value to existing and future data collections. A long-term added value in the significant reduction of development times of new processes and materials. The presentation will present first results of a new iBain, conducted within the German research initiative Material Digital.



**20:00 Invited**

**Influence of the Mobilities of Triple Junctions and Grain Boundaries on the Kinetics of Grain Growth**

*Ernst Gamsjaeger<sup>1</sup>; Jiri Svoboda<sup>2</sup>; <sup>1</sup> Montanuniversitaet Leoben; <sup>2</sup>Academy of Sciences of the Czech Republic*

The kinetics of grain growth is investigated for an idealized two-dimensional, periodic grain arrangement represented by one four-sided grain, two six-sided grains and one eight-sided grain. The grain boundaries might lengthen or shorten during grain growth. This process is taken into account by an automatic remeshing tool, continuously generating and eliminating node points of the arrangement. A finite mobility is assigned to each triple junction. A certain grain boundary energy and mobility is attributed to each grain boundary. It is shown that regions of small mobilities of triple junctions and grain boundaries may enhance the increase of the area of the eight-sided grain. Thereby, locally pinned triple junctions and grain boundaries may provoke abnormal grain growth. These numerical investigations are qualitatively compared to results from optical micrographs of microalloyed steel samples. Normal grain growth is attributed to the microstructure of fine austenite grains at a low soaking temperature (less or equal 1000°C) and to coarse austenite grains at a high soaking temperature (more or equal 1200°C). A bimodal size distribution indicating abnormal grain growth occurs at medium temperatures (approximately 1100°C), Largely elongated grains occur where the grain growth is controlled by reduced mobilities of triple junctions.

**20:30 Invited**

**Mean-field Modelling of Heterogeneous Precipitation**

*Manon Bonvalet Rolland; The Royal Institute of Technology*

Inducing the formation of secondary particles is one of the most powerful manufacturing techniques for strengthening a material and is widely used in steels, nickel-base and aluminum alloys, for instance. Manufacturing or service can also lead to the formation of detrimental precipitates, like the embrittling sigma phase. Prediction of the kinetics of the transformation of these phases, desirable or undesirable, is

therefore highly important. This is possible, using mean-field approaches, when kinetic and thermodynamic databases are available and when the situation is simple enough, i.e. homogeneous precipitation. However, there is an increasing demand for treating more complex cases, for instance heterogeneous precipitation, where the local environment affects the transformation. Thus, new mean-field models for treating the enhanced precipitation at grain boundaries, the precipitation on deformation-induced dislocations or the sequential precipitation on precursor phases have been developed and will be introduced. In addition, results of the coupling of some of those models together with physically-based microstructure modelling tools for predicting the effect of hot working on the microstructure evolution will be presented.

**21:00 Break**

**Phase Field Modelling I**

**Chairs: TBD**

**21:15 Invited**

**The Sharp Phase Field Method: FFT-based Mechanical Solvers for Abrupt Interfaces and a Multiphase-field Extension**

*Alphonse FINEL<sup>2</sup>; Ahmed DIMOKRATI<sup>1</sup>; Yann LE BOUAR<sup>2</sup>; <sup>1</sup>Cadi Ayyad University; <sup>2</sup>Laboratoire d'Etude des Microstructures (ONERA-CNRS)*

Recently, a new phase field formulation has been proposed, the Sharp Phase Field Method (S-PFM) in which interfaces are resolved with only one grid point with no pinning on the grid and accurate rotational invariance, allowing to reduce the computational time by almost three order of magnitudes [1]. We will discuss two important points regarding the use of sharp interfaces. In most microstructures of interest, elastic fields are involved (precipitates with specific eigenstrains, cracks, voids, dislocations). The modelling of these microstructures with sharp interfaces requires the use

of accurate mechanical solvers that do not display oscillations. We therefore developed new FFT-based mechanical solvers that are mathematically stable and therefore free of any instability, even in the presence of stress singularities. Often, the modelling of microstructures requires the introduction of several phase fields to account for different phases or differently oriented variants of the same phase. Therefore, we developed a multi-field version of S-PFM. We illustrate this method through the analysis of grain growth and show that the kinetics of junctions between the sharp interfaces is accurately reproduced, even though these junctions are resolved by exceedingly few points (essentially a single point in a 2D setting).

### 21:45 Contributed

#### Phase-field Modeling of Microstructural Development During Bearing Steels Processing

*Farnaz Aghebatil; J. A. Mathews<sup>1</sup>; M. G. Mecozzi<sup>1</sup>; R. H. Petrov<sup>1,2</sup>; J. Sietsma<sup>1,2</sup>; <sup>1</sup>Delft University of Technology; <sup>2</sup>Gent University*

To comply with the higher demand for sustainable and energy-efficient technologies, wind turbines are being scaled up both in size and power. This increase in size and power urges for components, particularly main shaft bearings, with higher load-carrying capacities. Main shaft bearings operate under significant fluctuating wind-induced forces, leading to complex load spectra in the bearings steels. To increase reliability and thus the efficiency of bearings, it is desired to monitor the degradation process and understand the drivers and mechanisms of material aging leading to rolling contact fatigue. High uniformity of the metallographic structure and components is required to obtain the designed fatigue life, but achieving uniformity remains a challenge as long as the microstructural processes are not completely understood. The purpose of this study is to provide insight into the effect of various upstream process parameters on the essential aspects of the non-uniform microstructure that affects the material performance so strongly, by taking advantage of computational materials science. In this work, phase field modeling of the microstructure formation is used to analyse the microstructure evolution during processing in order to obtain an optimal microstructure, and likewise properties, by tailoring the manufacturing process. The

emphasis in this study is on the influence of cooling rate on bainite/martensite band formation. In order to demonstrate the mechanism involved in this process, the cooling process, the associated phase transformations, and the grain growth are simulated using the MICRESS software (MICROstructure Evolution Simulation Software). The resulting microstructures are analyzed quantitatively and compared with experimentally observed ones.

### 22:00 Contributed

#### Role of Solute Drag on the Phase Transformation Kinetics: A Phase-Field Study

*Ayush Suhane<sup>1</sup>; Hocine Lebbad<sup>1</sup>; Matthias Militzer<sup>1</sup>; <sup>1</sup>University of British Columbia*

To optimize alloy design and thermo-mechanical treatments in steels, advancement of knowledge regarding the kinetics of austenite-ferrite phase transformations is crucial. Alloying elements can significantly affect the transformation kinetics by segregating at the interfaces which reduces their migration rates due to solute drag. Recent experimental and modeling strategies have been able to successfully characterize the solute drag effect of a number of substitutional solutes (e.g. Mn, Ni, Si, Cr) in ternary Fe model alloys. The reduction in interface velocity is frequently rationalized using a phenomenological binding energy for each solute. However, its equivalence to solute-interface interactions occurring at the atomistic length scale remains a challenge. Furthermore, the current numerical models are limited by their application to planar interfaces operating under steady-state growth conditions.

The present work aims at overcoming these two limitations for describing phase transformation kinetics. We propose a phase-field model (PFM) to assess the effect of solutes on the interfaces under non-steady state growth conditions. First, the model is benchmarked against the standard Cahn's continuum model for grain growth. An alternative approach is proposed to evaluate the phenomenological binding energy from density functional theory simulations. From the atomistically obtained binding energies, the total enrichment at the interface has been estimated and has been seen to capture the magnitude of solute drag pressure as opposed to the peak binding energy. Extension of the model to simulate austenite to ferrite phase transformation in a binary Fe-Mn

alloy confirms the role of Mn in the reduction of the austenite-ferrite transformation temperatures typically observed in continuous cooling experiments.

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*2022*

Wednesday | 29 JUNE 2022 GMT+8 (Beijing)

**Zoom link:****Chairs:****16:00 Plenary****Chemical Patterning of Alloys***[Christopher Hutchinson](#); Monash University*

Phase transformations are one of the most powerful means we have to manipulate the microstructures of engineering alloys with the goal of achieving improved combinations of properties. It is usually desired that these phase transformations occur from a reasonably chemically homogenous parent phase. The rationale is that this will lead to a more homogenous microstructure after transformation. Chemical heterogeneities in the parent phases, such as banding in steels, is usually discouraged. However, the microstructures of our most advanced metallic materials are becoming more and more heterogeneous, and in particular, advanced steels may contain a number of different phases, with different fractions, arranged carefully to deliver the impressive combinations of mechanical properties they exhibit. These complex microstructures can benefit from a parent phase that is chemically patterned in a controlled way.

In this talk, I discuss moving away from the ideal of a chemical homogenous template on which subsequent phase transformations occur and discuss examples of creating deliberately chemically patterned parent phases. Two examples are discussed. The first uses the partitioned pearlite reaction in alloyed steels followed by re-austenitization to create a Mn chemical pattern in the austenite which can then form a nanolaminate of martensite and austenite on cooling. The second example considers laser powder bed fusion (3D printing) of mixed powders designed to provide melt pools of different chemistries to select different phases during solidification. Both cases exploit deliberate chemical heterogeneity in the parent phases to create new types of microstructures through phase

transformations and allow access to new combinations of properties.

**17:00 Break****21:00 Plenary****A Pair of New Developments of Phase-field Method for Solid-State Phase Transformations***[Long-Qing Chen](#); The Pennsylvania State University*

Phase-field method is a density-based computational approach at the mesoscale for modeling and predicting the temporal microstructure and property evolution during materials processes. The presentation will start with a brief introduction to the thermodynamic basis of the phase-field method [Prog in Mater Sci, 2022, 124: 100868]. The focus of the presentation will be on two of our recent efforts in advancing phase-field method of solid-state phase transformations and the accompanying morphological pattern formation. The first is a phase-field model of phase transformations involving perfectly ordered stoichiometric compounds [Acta Mater 2022, 118007]. Essentially all existing phase-field models treat stoichiometric compounds as disordered solid solutions by approximating their mathematically delta-function dependences on composition with parabolas assuming a rather arbitrary curvature, leading to possibly orders of exaggerated non-stoichiometries, thermodynamic inconsistencies, and numerical instabilities. Our recent phase-field model of homogeneous and heterogeneous stoichiometric reactions avoids the use of the parabola approximation of stoichiometric compounds. It offers a straightforward connection to existing thermodynamic databases containing a combination of multiple stoichiometric and solution phases. This model is generally applicable to many common processes such as precipitation of stoichiometric and solution phases in multicomponent alloys, crystallization of stoichiometric compounds, vapor-phase deposition of stoichiometric thin films or two-dimensional materials, oxidation of alloys, electrochemical deposition, interfacial reactions, etc. The second is a class of phase-field models of mesoscale



structure evolution during concurrent structural and electronic processes in functional and quantum materials. Examples include electronic phase separation [PRB, 2020. 102(19): 195101], simultaneous metal-insulator and structural phase transitions [PR Materials, 2018. 2(5):053803; PR Applied, 2019. 11(1); PRB, 2021. 104(6): 064308; Science, 2021. 373(6552): p. 352; PR Applied, 2022. 17(1): 014042] ferroelectric phase transitions and domain dynamics accompanied by elastodynamics [PRL 2020. 124(10): 107601; PRB, 2021. 103(22): L220303] and electronic carrier evolution [npj Comp Mater, 2022: Accepted], and thermally ultrafast electron and lattice relaxation processes in strongly correlated systems with co-existing electronic, spin, and lattice orders [2022]

## Zoom Room A

### Bainite and Martensite II

Zoom link: TBD

Chairs: TBD

#### 17:15 Invited

#### Discontinuous Martensite Transformation Kinetics in a Low Carbon Steel Tailored by Annealing Twins in Austenitic Parent Phase

*Yongchang Liu<sup>1</sup>; Chunliang Mao<sup>1</sup>; Chenxi Liu<sup>1</sup>; <sup>1</sup>Tianjin University*

Martensite transformation in low carbon steel will relate to the discontinuity of the martensite transformation rate, which exhibited a series of martensite transformation rate peaks, especially in low cooling rate. Although some authors reported the above phenomenon, but all of them either simply presented the martensite transformation rate is gradual without depth analysis or presented some controversial conclusions with each other. Here emphasis was paid on the correlation of the discontinuity of the martensite transformation rate and annealing twin in parent austenite grain in a low carbon reduced activation ferritic/martensitic (RAFM) steel. Through combining dilatometer, in-situ high temperature laser confocal scanning microscope

(LSCM) and parent austenite reconstruction basing on electron backscatter diffraction (EBSD) technology, we concluded that the not only the lath martensite microstructure is hierarchical but also the lath martensite transformation rate peaks are hierarchical in chronological order. If the cooling rate was not too high, initially, the lath martensite transformation rate peaks will be divided into two groups by annealing twin in parent austenite. These transformation rate peaks in the first group were mainly caused by the lath martensite transformation, which occurred in the non-twin zone of the parent austenite grain. Then, the second group was mainly consisted of a single transformation rate peak with a high full width of half maximum (FWHM), which was mainly caused by the martensite transformation in the twin zone in parent austenite grains. This classification mechanism was discussed in the present work. The relationship between twin in parent austenite grains and martensite packets was also studied by EBSD. Twin can evolve into a martensite single packet in the process of lath martensite transformation.

#### 17:45 Contributed

#### Experimental Investigation and Modeling of Microstructural Evolutions during the Tempering of Martensitic and Nano-bainitic Low-alloyed Steel

*Steve Gaudes<sup>1</sup>; Sabine Denis<sup>1</sup>; Julien Teixeira<sup>1</sup>; Guillaume Geandier<sup>1</sup>; Benoit Denand<sup>1</sup>; Jaafar Ghanbaja<sup>1</sup>; Thomas Sourmail<sup>2</sup>; Matthias Kuntz<sup>3</sup>; Sebastien Allain<sup>1</sup>; <sup>1</sup>CNRS-Universite de Lorraine; <sup>2</sup>ASCO metal CREAS; <sup>3</sup>Robert BOSCH GmbH*

"Nano-structured bainite microstructures have been recently introduced to design new classes of low-alloyed steels. Nano-bainite is obtained after isothermal transformation at low temperature (150-300°C) for times of the order of 24 h. Nanostructured bainite is composed of thin carbon super-saturated bainitic ferrite laths (ca. 40 nm) and high fraction (up to 40 wt.%) of retained austenite [1], conferring high ductility and tensile strength to these steels. Tempered nano-bainite microstructures also exhibit resistance to softening comparable to tempered martensite microstructures with secondary hardening [2]. This gives the possibility to combine nano-structured bainite and secondary hardening

precipitation in order to target applications for fatigue resistance in higher temperature range. A project is ongoing in this framework to design a new class of steel, taking as a basis one nano-bainitic steel grade previously investigated (0.67C-1.7Si-1.7Cr-1.3Mn wt.%). Mo (1wt.%) and V (0.5wt.%) elements are added to enable secondary carbide precipitation.

The aim of this study is to investigate experimentally and to simulate the microstructural evolutions during the tempering of this nano-bainitic steel. We highlight here the difference with the precipitation sequence occurring during the tempering of martensitic steels, which is well documented [3]: precipitation of transition carbides is followed by cementite precipitation, austenite decomposition and finally the precipitation of alloyed (secondary) carbides. Differences in nano bainitic steels are the initial ferrite matrix and the large fraction of austenite. The experimental approach is based on the investigation of three different initial microstructures: nano-bainite, martensites quenched at room temperature or in liquid nitrogen. Aim of the two quenches is to make vary the austenite fraction, a key feature of nano-bainitic steels. The sequences of microstructural evolutions during the tempering were followed by complementary experimental techniques including hardness, dilatometry and in situ synchrotron. High energy X-rays diffraction (HEXRD) is introduced as an original experimental method to track in situ and quantitatively the precipitation sequences and the evolutions of the matrix phases bainitic ferrite/martensite and austenite phase fractions during the tempering. Conventional techniques including hardness measurements, dilatometry, electrical resistivity, microstructure characterization by TEM are employed in addition. Combined to these experiments, physical-based modeling of the precipitation sequence is carried out in order to assess the thermokinetic analysis by comparing the quantitative predictions to experimental data. First outcomes are from the in situ HEXRD experiments, which provide the mass fraction evolutions of not only the matrix phases (ferrite/martensite, austenite), but also the low-amount precipitate phases (transition carbides, cementite and secondary carbides), giving their respective kinetics of formation and dissolution. The studied steel presents a non-expected high stability of the retained

austenite against decomposition for both martensitic initial microstructures as well as nano-bainite. The evolutions of the lattice parameters in martensite and bainitic ferrite are discussed considering the issue of the carbon supersaturation in these systems. Carbon composition of the austenite is another key parameter as it determines the amount of solute available for precipitation. Micromechanical analysis is introduced for full interpretation of cell parameters evolutions. In addition, Williamson-Hall analysis is performed to establish the recovery kinetics during tempering. From TEM combined with EDS, it is shown that the cementite starts to form without partition. It then enriches in Mn, Cr and depletes in Si as expected from thermodynamics. More complex evolutions regarding Mo and V due to the interaction with the MC precipitation and retained austenite are evidenced.

The nucleation and growth model with physical basis developed is based on a previous work [4]. It now considers the secondary precipitation, the presence of the retained austenite and its decomposition, different hypotheses such as cementite nucleation and first growth stages without partition, and improved modeling of dislocation recovery. The precipitation kinetics, the carbides densities, radii and composition evolutions are predicted considering their interactions (interactions cementite and MC carbides), together with the evolutions of the matrix phases. The quantitative predictions are compared to experiments. Finally yield strength is predicted on a physical basis as a function of the precipitation state, for the future purpose of alloy composition and thermal treatment design.

References: [1] Caballero, F.G. et al., *Materials science and technology*, 18(3), pp.279-284. [2] Garcia-Mateo, et al., *Materials Science and Technology*, 20(7), pp.814-818. [3] Krauss, G., 2012., *Phase Transformations in Steels* (pp. 126-150). Woodhead Publishing. [4] Wang, Y., et al., *Journal de Physique IV (Proceedings)* (Vol. 120, pp. 103-110). EDP sciences.

**18:00 Contributed**  
**Effect of Free Surface on Low Temperature Formation of Martensitic-Bainitic Microstructures**

*Alfonso Navarro-Lopez<sup>1</sup>; Javier Hidalgo<sup>1,3</sup>; Goro Miyamoto<sup>2</sup>; Tadashi Furuhashi<sup>2</sup>; Jilt Sietsma<sup>1</sup>; Maria J. Santofimia<sup>1</sup>; Alfonso Navarro-Lopez<sup>1</sup>; <sup>1</sup>Delft University of Technology;<sup>2</sup>Tohoku University;<sup>3</sup>Universidad de Castilla-La Mancha*

The continuous development of advanced multiphase steels with increasingly outstanding mechanical performance has enabled the thickness reduction of steel components used for structural applications. The use of thin steel sheets makes it necessary to consider the effects derived from a free surface in the development of microstructures. Free surface effects are expected to create a microstructure-properties gradient along the thickness of the steel sheet with consequences in the final performance of the component. The present research investigates the free surface effects on phase transformations involved during low temperature isothermal treatments in a low-carbon high-silicon steel. Surface observations by in-situ laser confocal microscopy in combination with theoretical thermodynamic calculations confirm that the strain energy needed for strain accommodation related to phase transformations is lower at the surface than in the bulk. Electron back scatter diffraction and dilatometry measurements enable the microstructural characterization of the distinct micro-constituents formed at the surface and within the bulk and their comparison in terms of phase nature (martensitic or bainitic), grain size, and growth direction.

**18:15 Break**

## Martensite

**Chairs: TBD**

### 19:15 Invited Characteristics of Nucleation and Transformation Sequence in Martensitic Transformation in SUS321 Stainless Steel

*Wei Xu<sup>1</sup>; Jinliang Wang<sup>1</sup>; Chenchong Wang<sup>1</sup>; <sup>1</sup>Northeastern University*

To elucidate the characteristics of the nucleation and

transformation of temperature-induced and deformation-induced martensitic transformation, detailed characterizations were performed during cryogenic treatment and quasi-in-situ tensile deformation. For temperature-induced martensitic transformation, a new viewpoint was proposed, that nucleation could occur on new defects generated during cryogenic treatment, and not just on pre-existing defects. Moreover, transformation processes for both  $\gamma \rightarrow \epsilon \rightarrow \alpha'$  and  $\gamma \rightarrow \alpha'$  routes, their associated mechanisms, and crystallographic characteristics were analysed in detail. For deformation-induced martensitic transformation, two possible transformation scenarios were simultaneously observed and investigated in detail.  $\epsilon$ -Martensite initiated within the shear band is the most preferential nucleation site instead of slip band intersections as assumed in the classical theory. The correlation between the two transformation sequences is discussed and associated with strain and stress conditions. Characteristics of the nucleation and transformation sequence upon deformation are compared to thermal martensitic transformation; systematic similarity is discovered, implying the underlying shared nature of thermal and mechanical stabilities.

### 19:45 Contributed Microstructure Characterization of Martensitic Materials by Differential Interference Microscopy System

*Zhuohui ZENG<sup>1</sup>; Hoi Chun CHIU<sup>1</sup>; Luwei ZHAO<sup>1</sup>; Teng ZHAO<sup>1</sup>; Chenbo ZHANG<sup>1</sup>; Mostafa Karami<sup>1</sup>; Wei GUO<sup>1</sup>; Shengwang DU<sup>1</sup>; Xian CHEN<sup>1</sup>; <sup>1</sup>Hong Kong University of Science and Technology*

Differential interference microscope can be applied to observe the surface topography of martensitic materials. From the differential interference image, we can distinguish different variants of martensite so that it is possible to study the evolution of microstructures and surface topography of martensitic materials with it. We can simultaneously investigate the microstructures and thermal behaviors during the martensitic transition of martensitic materials and also precisely determine the beginning/ending moment of the phase transformation with the help of differential interference optical system and differential scanning

calorimetry machine. A mathematical model by which the topography and the deformation of the martensitic microstructure are quantitatively determined by the reflected light differential interference microscopy technique has been proposed by us. Firstly, the optical parameters of the differential interference microscope are determined with a standard sample. Secondly, based on the mathematical model, we conduct a measurement to demonstrate the determination of the surface relief of microstructure comprised of a pair of twinned martensitic variants. The surface height gradients of the martensitic twin, which are two martensite variants, along the beam-shear direction of differential interference microscope agree well with the values measured by the atomic force microscopy. By comparing the measurements of atomic force microscopy and differential interference microscope, the current microscopy system can resolve the microstructures with the fineness of around 500 nm, and it measures the surface slope with 0.005 rad accuracy. We also develop a dual beam-shear DInC optical system which can detect the surface height gradient in two perpendicular directions within 100ms so that we can in-situ detect the microstructures evolution of martensitic transformation. Combining with digital image correlation technics, dynamic behaviors of a local area on poly-crystalline NiTi and single-crystalline AuCuZn during the martensitic transformation have been recorded. We observe a local height gradient jump during the phase transformation of NiTi but there is no such a jump in the AuCuZn sample which satisfies the cofactor conditions. This presentation underlies a new approach for quantitative surface topography determination with wide applications in experimental mechanics.

**20:00 Contributed**

**In-situ X-ray Diffraction Study on the Effect of Cooling Rate on the Martensitic Transformation in High Carbon Steels**

*Thomas Kohne<sup>1</sup>; Peter Hedstroem<sup>1</sup>; Annika Borgenstam<sup>1</sup>; <sup>1</sup>KTH Royal Institute of Technology in Stockholm*

The cooling rate after austenitization has been shown to have a strong impact on the fatigue performance of case-hardened steels with differences of up to 20 %. The mechanism/s for this increase is not fully understood, but a correlation

between dilatometer results for a high carbon steel with composition close to the surface composition of the case-hardened material and the fatigue performance was observed. To clarify the underlying mechanism/s the effect of cooling rates on the martensitic transformation in high carbon steel was studied with a special emphasis on the transformation kinetics and final microstructure. In-situ high energy x-ray diffraction (HEXRD) and dilatometer tests were used for the study of transformation kinetics combined with analysis of the final microstructure that consists of martensite and retained austenite by electron microscopy, mainly electron backscatter diffraction (EBSD). The combination of results are presented here and the possible mechanisms governing the enhanced fatigue performance are discussed.

**20:15 Contributed**

**Characterization and Crystallographic Analysis of Lath Martensitic with Greninger-Troiano Orientation Relationship in a Fe-12Ni-1.5Si-0.2C Steel**

*Duanjun Sun<sup>1</sup>; Zhenghong Guo<sup>1</sup>; Jianfeng Gu<sup>1</sup>; <sup>1</sup>Shanghai Jiao Tong University*

A novel austenite reconstruction technology was developed to reveal the prior austenite grains when there is little retained austenite or only the orientation of martensite was known by EBSD observation. Then an optimal scheme based on clustering algorithm was proposed to determine the orientation relationship between prior austenite and martensite quantitatively. For Greninger-Troiano relation found in the present Fe-12Ni-1.5Si-0.2C steel, detailed characterizations about crystallographic features were carried out. Results show that three crystallographically distinct blocks with the common  $\{111\}_\gamma$  interface were configured into a packet with self-accommodation manner to minimize macro strain, and three slip systems of dislocations with  $\langle 111 \rangle_{\alpha'}$  Burgers vectors were involved during the martensitic transformation. Regarding these information and selecting the bivariant block as the basic element which undertakes the invariant plane shear, the modified version of crystallographic model was proposed to clarify the microstructural evolution phenomenologically.

**20:30 Contributed**



### Martensitic Transformation Mechanism of Pre-deformed Austenite during Continuous Cooling to 4 K – competing Effects between Slip Band Density and Spacing

*Dong Guangqi<sup>2</sup>; Jinliang Wang<sup>1</sup>; Chenchong Wang<sup>2</sup>; Jun Hu<sup>2</sup>; Lingyu Wang<sup>2</sup>; Wei Xu<sup>3</sup>; <sup>1</sup>Guangdong Ocean University; <sup>2</sup>Northeastern University*

Plastic deformation of metastable austenite has long been regarded as a source of mechanical stabilization that makes austenite less susceptible to temperature induced martensitic transformation during cooling. However, it is also documented that small deformations below 5% seems to promote martensitic transformation and increase the final martensite content at the end of the cooling process. Little knowledge was established in the transformation kinetics and underlying mechanisms that cause this transition in austenite stability. In this contribution, we use magnetic measurement during continuous cooling to measure the transformation kinetics of pre-deformed austenite down to 4 K and provide microstructural evidence on the determining factors that tunes the austenite stability. While small deformation provides more slip bands serving as extra heterogeneous nucleation sites, large deformation reduces the spacing between slip bands which suppress the further growth of martensite. The density of defects and their spacing determine their promoting/suppressing effect on martensitic transformation.

**20:45 Break**

**Zoom Room B**

### Additive Manufacturing II

**Zoom link: TBD**  
**Chairs: TBD**

### 17:15 Invited Strategies for the Design of Steels for Additive Manufacturing

*Pedro Rivera-Diaz-del-Castillo<sup>1</sup>; Hossein Eskandari Sabzi<sup>1</sup>; <sup>1</sup>Lancaster University*

Additive manufacturing requires the development of novel steel grades displaying both printability and attractive mechanical properties. Printability can be embodied by crack prevention and pore/void minimisation strategies, whereas attractive mechanical properties include strength, ductility and toughness. In this presentation two families of alloys are considered, stainless and maraging steels. Crack prevention is ensured by controlling the solidification path, promoting or inhibiting phases such as ferrite, which is desired upon solidification of austenitic stainless but avoided in maraging steels. The solidification path can be controlled via adopting thermodynamic criteria directly linked to composition. Porosity is instead controlled through tailoring the melt pool geometry, and by imposing limits to the energy input with respect to the enthalpy of melting; the later is composition and process dependent. Post-treatment steps are required to tailor precipitation hardening in maraging steels. The complexity of the problem requires sophisticated thermodynamic and kinetic calculations; these are combined with genetic algorithms to find novel alloy grades combining the desired printability and improved properties. Examples are introduced in 316L-type stainless steels, and Cu nanoprecipitate-hardened maraging grades.

### 17:45 Contributed Micro-cell and its effects on Austenite Reversion in Selective Laser Melted Maraging Steels

*Yingjie Yao<sup>1</sup>; Ran Ding<sup>1</sup>; Xiaosheng Zhou<sup>1</sup>; Wei Liu<sup>1</sup>; Zhigang Yang<sup>1</sup>; Chi Zhang<sup>1</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>Tsinghua University*

The micro-cell is a unique microstructure in alloys additively manufactured by selective laser melting (SLM). It was widely accepted that the boundaries of micro-cells are zones with a high dislocation density and chemical segregation in SLMed alloys without solid-state phase transformations. However, the present study indicates that there is only chemical segregation but no dislocation network at cell boundaries of the SLMed maraging steels. We deduced the dislocation network may be formed during the rapid solidification, while it was removed by the cyclic  $\gamma \leftrightarrow \alpha'$ ; solid-state phase transformations during additive

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manufacturing. The micro-cells in the SLMed maraging steels were also found to significantly alter austenite reversion and precipitation behavior during the post aging process. It was interestingly found that the micro-cell boundaries could serve as preferential sites for austenite reversion during aging of the SLMed steels, constructing a three-dimensional metastable austenite network. The micro-cell opens a new route to architect novel microstructures in additive manufactured alloys.

**18:00 Contributed**

**The effects of Solidification Process Parameters on Yield Strength in Laser Powder Bed Fusion**

*Hossein Eskandari Sabzi<sup>1</sup>; Pedro Rivera-Díaz-del-Castillo<sup>1</sup>; <sup>1</sup>Lancaster University*

Alloys made by additive manufacturing (AM) have attracted increasing interest in recent scientific research, due to the unique freedom of design offered by AM technologies. Laser powder bed fusion (LPBF) is one type of AM technology, which has gained much popularity due to its versatility in fabricating various important engineering alloys such as 316L stainless steel, IN718 and Ti-6Al-4V. The energy transferred to the powder bed to melt the powder in LPBF process can be expressed by the normalised enthalpy, which relates the LPBF process parameters such as laser power, scan speed laser spot size to the thermodynamic features of the material to be printed such as laser absorptivity, enthalpy of melting, thermal conductivity, density and heat capacity. Solidification-induced strains are dictated by the normalised enthalpy leading to a chain of softening and hardening mechanisms such as dislocation multiplication/annihilation and phase transformations that affect the yield strength of LPBF processed components. In this work, the yield strength of fully-dense LPBF components made from 316L stainless steel, IN718 and Ti-6Al-4V is predicted, considering different contributions of thermally-activated phenomena. It is therefore demonstrated that, in the as-built condition, solidification thermodynamic parameters can be directly employed for describing strengthening of LPBF components. The theory shown here can guide alloy and microstructure design of new AM products.

**18:15 Break**

**Additive Manufacturing III**

**Chairs: TBD**

**19:15 Invited**

**2D and 3D EBSD Studies of Variant Selection during Electron Powder Bed Fusion of Ti-6Al-4V**

*Sophie Primig<sup>1</sup>; Sophie Primig<sup>1</sup>; <sup>1</sup>UNSW Sydney*

Ti-6Al-4V is one of the most commonly used alloys for additive manufacturing (AM) due to its applications as orthopaedic implants and aerospace components which can uniquely benefit from the advantages of AM. However, the inherent inhomogeneity and cyclic thermal loading in additive manufacturing processes significantly complicate the microstructural evolution of this alloy. The current understanding of the microstructural evolution in Ti-6Al-4V is based on traditional processing and cannot adequately predict its behaviour during AM. Analysis of different interfaces (prior beta grain boundaries, alpha inter-variant boundaries) formed during AM of Ti-6Al-4V can clarify the competition between different modes of alpha variant selection in determining the final microstructure. Here, traditional 2D characterization methods are often insufficient for uncovering complex, interconnected microstructural features that arise from solid-solid phase transformations during AM. In this work, Ti-6Al-4V blocks were produced using different scanning strategies during electron beam powder bed fusion and characterized using 2D and 3D electron backscatter diffraction. This revealed that the microstructure is more complex, and that alpha laths are more interconnected than previously believed. For example, inter-variant boundary character distributions showed significant evidence of different variant selection mechanisms as a function of the position in the build and the scanning strategy. Some of these variant selection mechanisms are more desirable than others. Understanding the complexity of the microstructure in 3D provides new insights into the fundamental phenomena behind the microstructural evolution of titanium alloys in AM, and will

help to give recommendations for optimising process design. Acknowledgements: Funding by the AUSMURI program, Department of Industry, Innovation and Science, Australia is acknowledged. Samples were provided by Prof. Suresh Babu and Miss Sabina Kumar, The University of Tennessee, Knoxville.

#### 19:45 Invited

#### Additive Manufacturing of Ultra-fine Grained, Pearlitic Titanium-copper Alloys

*Dong Qiu<sup>1</sup>; Duyao Zhang<sup>1</sup>; Mark Easton<sup>1</sup>; <sup>1</sup>RMIT University*

Pearlite is one of the most classic microstructures in ferrous alloys, combining excellent strength and fracture toughness. Titanium also involves a pearlitic reaction with certain alloy elements (e.g. Cu, Fe and Ni). However, the addition of these eutectoid forming elements to titanium is strictly restricted in practice due to the high susceptibility of microsegregation that deteriorates the mechanical properties. Therefore, pearlitic titanium alloys have received little attention compared to ( $\alpha + \beta$ ) or metastable  $\beta$ -Ti alloys. The rapid development of metal additive manufacturing technologies offers a great opportunity to solve this long-standing problem. In this paper, a series of Ti-xCu alloys ( $x = 3.5\text{wt}\%$ ,  $6.5\text{wt}\%$  and  $8.5\text{wt}\%$ ) were fabricated through laser metal deposition (LMD) process. The as-fabricated samples do not show any noticeable segregation across the grain boundary or layer boundary. This is because the intrinsic high cooling rate in the LMD process leads to very fine dendrites and restrict the segregation to the scale of a few micrometres or below. Then subsequent multiple thermal cycles can homogenize the compositional variation efficiently through a dynamic annealing effect. In addition, the LMD process provides a much higher cooling rate than that of conventional normalizing process and hence enables much finer inter-lamellae spacing ( $\sim 45 \text{ nm}$ ) in the as-fabricated Ti-8.5wt%Cu alloy. The kinetics of eutectoid decomposition and microstructure evolution during the complex thermal cycles is also discussed at different locations along the building direction. It is anticipated that this work can be equally applicable to other eutectoid forming alloy systems and contribute to the development of high-performance pearlitic alloys by taking the full

advantage of metal additive manufacturing technologies.

#### 20:15 Contributed

#### Phase Transformation during Heating in Ti64 Alloy Elaborated by Powder Bed Fusion

*Moukrane Dehmas<sup>1</sup>; Charlotte Dupressoire<sup>2</sup>; Joel Alexis<sup>3</sup>; Jonathan Hugues<sup>2</sup>; Antonio Castro Moreno<sup>2</sup>; <sup>1</sup>CIRIMAT; Université de Toulouse; <sup>2</sup>IRT Saint Exupéry; <sup>3</sup>Université de Toulouse*

As titanium-based alloys possess interesting specific mechanical properties, they are increasingly used in aerospace industry. Additive manufacturing is able to produce complex near net shape parts reducing the raw material quantity involved. This potential is of great interest for industrial applications. Among additive manufacturing processes, powder bed fusion technologies are the most widespread. Depending on the energy source, Laser Beam Melting (LBM) and Electron Beam Melting (EBM) processes are distinguished. However, even if these new ways of elaboration offer several advantages, there is a lack of knowledge about materials properties. The microstructure inherited from LBM and EBM needs to be finely characterized to understand its response to heat treatment. This will lead to the determination of alternative heat treatments specific to additive manufacturing processes. This study was performed on Ti64 alloy, elaborated by LBM and EBM. For LBM, fine  $\alpha'$  martensite is observed whereas EBM components offer  $\alpha/\beta$  lamellar microstructure. Microstructure and crystallographic texture of as-fabricated alloy were characterized and determined using Scanning Electron Microscopy (SEM) and Electron BackScattered Diffraction (EBSD), respectively. Electron Probe Micro Analysis (EPMA) was used to determine local chemical composition and to reveal the presence of chemical segregations inherited from fast solidification occurring during process. In addition, phase transformation sequences were studied on heating thanks to dilatometry, in situ electrical resistivity and high energy synchrotron X-ray diffraction to reveal the effect of heterogeneous microstructure. A comparison with Ti64 alloy manufactured by conventional processes is proposed.

#### 20:45 Break

## Zoom Room C

## Titanium Alloys II

Zoom link: TBD

Chairs: TBD

## 17:15 Invited

**Mechanisms of Beta-to-omega and Omega-assisted Alpha Phase Formation in near Beta-titanium Alloys**

*Tong Li<sup>1</sup>; Damon Kent<sup>2</sup>; Gang Sha<sup>3</sup>; Anna Ceguerra<sup>4</sup>; Matthew Dargusch<sup>5</sup>; Julie Cairney<sup>4</sup>; <sup>1</sup>Institute for Materials; <sup>2</sup>University of Sunshine Coast; <sup>3</sup>Nanjing University of Science and Technology; <sup>4</sup>The University of Sydney; <sup>5</sup>The University of Queensland*

Near  $\beta$ -Ti alloys often utilise a dispersion of the  $\omega$  phase to nucleate even  $\alpha$  precipitation, enhancing the properties of the alloy. However, the form and conditions of  $\omega$  which assist  $\alpha$  precipitation remain unclear in the literature. In this study, we employed aberration-corrected TEM and atom probe tomography and a specifically-developed APT algorithm to study  $\alpha$  precipitation in alloys designed to contain two different types of  $\omega$ . Here we found out that incommensurate embryonic  $\omega$  does not directly assist  $\alpha$  precipitation. When it reaches a critical size, it transforms to isothermal  $\omega$ , which stimulates the formation of  $\alpha$ . We also discuss the dominant factor in each transformation step, i.e. the release of coherency strain at a critical size is the dominant factor for the transformation from embryonic  $\omega$  to isothermal  $\omega$ , and O enrichment at semi-coherent  $\omega/\beta$  interfaces possibly plays the key role in controlling the precipitation of  $\alpha$ .

## 17:45 Contributed

**Variant Selection Rules for Grain Boundary Alpha in A Metastable Beta-Titanium**

*Renlong Xin<sup>1</sup>; Yu Zhang<sup>1</sup>; Xiaowei Lan<sup>1</sup>; Renlong Xin<sup>1</sup>; <sup>1</sup>Chongqing University*

The final mechanical properties of titanium alloys are strongly influenced by  $\beta$ -transformed microstructures, especially the morphology and crystallographic orientation

of  $\alpha$  phase. During cooling from the  $\beta$  field, the  $\alpha$  phase first precipitates at the prior  $\beta$  grain boundaries (GBs) and maintains the Burgers orientation relationship (BOR) with one of two adjacent  $\beta$  grains. This GB  $\alpha$  layer is considered as the origin of low ductility, leading to intergranular fracture. Therefore, it is crucial to figure out the crystallography of GB  $\alpha$  and its variant selection rules. In this talk, five parameters of GBs in a TB8 alloy were determined by combined use of electron backscatter diffraction (EBSD) and focused ion beam (FIB) techniques. Then, a systematic investigation regarding the use of multiple variant selection rules including the effect of both misorientation and grain boundary plane (GBP) inclination was carried out. The results suggested that rule 1 based on the double BOR could shortlist candidates among 24 possible variants when disorientation angle  $\theta_m < 10^\circ$ . To further refine data predicted by rule 1, five additional rules dealing with arrangement of GBP were also analyzed. Overall, the combined use of empirical rules looks promising for predicting which variant to select at prior  $\beta$  GBs.

## 18:00 Contributed

**Significant Enhancement of High Temperature Oxidation Resistance of Pure Titanium via Minor Addition of Nb and Si**

*Zhangzhi Shi<sup>1</sup>; Xu Jun-Yi<sup>1</sup>; Liu Xue-Feng<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing*

A novel Ti-0.5Nb-0.5Si (in wt.%) alloy is oxidized at 650~850 °C for 100 h in air, which shows a significant higher oxidation resistance than pure Ti. The advantage of the alloy becomes more obvious with increasing temperature. At 850 °C for 100 h, mass gain of the alloy only accounts for 12.7% of that of the pure Ti. A key reason is the formation of a Ti<sub>2</sub>N layer coherent with Ti matrix. At the scale/substrate interface of the alloy, there forms a Ti<sub>2</sub>N layer coherent with  $\alpha$ -Ti matrix, which acts as a barrier for oxidation. They exhibit an OR of (001)Ti<sub>2</sub>N//[(11-20)Ti, [1-10]Ti<sub>2</sub>N// [1-10-1]Ti. The degree of their coherency can be described by 50% of  $\alpha$ -Ti lattice points matching perfectly with 100% of Ti<sub>2</sub>N lattice points, or 1/4 atoms in Ti crystal matching perfectly with 1/6 atoms in Ti<sub>2</sub>N crystal. So an interface between them will have low energy, which



provides strong adhesion of the scale to the substrate. The oxide scale of the alloy with less porosity and alleviated stratification creates an environment at the scale/substrate interface favorable for the formation of Ti<sub>2</sub>N.

## 18:15 Break

## Interfaces

Chairs: TBD

### 19:15 Invited Quantitative Electron Tomography with Applications to Studying Aluminum Alloys

*Jianghua Chen; Hunan University*

Developments of high-strength aluminum alloys have always faced a difficult problem: owing to their small size, the early-stage strengthening precipitates are difficult to characterize in terms of composition, structure and evolution. Here we employ atomic-resolution transmission electron microscopy (TEM) imaging and first-principles energy calculations to address these problems. Recent years, we have investigated tens of typical high strength aluminum alloys, such as 2xxx (AlCu, AlCuMg and AlCuLiMg), 6xxx (AlMgSi and AlMgSiCu) and 7xxx (AlZnMg and AlZnMgCu) alloys, with different compositions and with varying thermal processes for understanding their property-structure-process correlations. Using aberration-corrected high-resolution TEM (HRTEM) and aberration-corrected scanning TEM (STEM), much of our attention has been paid to revisit the strengthening precipitates in these important alloys and to clarify the controversies left in the past about their precipitation behaviors. Our study demonstrates the followings: (1) Atomic-resolution imaging in STEM can provide straightforward structure models at the atomic-scale, whereas atomic-resolution imaging in HRTEM with rapid quantitative image simulation analysis can provide the refined structures with high precision beyond the resolution limitation of the microscope. The combination of the two techniques can be more powerful in solving difficult structure problems in materials science. (2) Most of the

early-stage precipitates in aluminum alloys are highly dynamic in both composition and structure. Typically, having their characteristic genetic skeletons to guide their evolution, these dynamic precipitates initiate, mature and grow with thermal aging following characteristic evolution paths. The fine precipitation scenarios revealed in our studies are rather different from previous understandings in the textbooks and literatures published thus far.

### 19:45 Invited Phase Transformation Interfaces: Past, Present and Future

*James Howe<sup>1</sup>; James Howe<sup>1</sup>; <sup>1</sup>University of Virginia*

This presentation will describe the use of both static and in-situ high-resolution (scanning) transmission electron microscope (S)TEM techniques to understand the mechanisms of phase transformations and the behavior of transformation interfaces at, or near, the atomic level. Examples will demonstrate how in-situ imaging and spectroscopic techniques can be used to quantify both the structural and compositional evolution, as well as the temporal dynamics, of transformation interfaces at temperature. Such data reveal insights into mechanistic aspects of transformation interfaces on time scales related to thermally activated, diffusional processes. Recent advances in detectors for both imaging and spectroscopy, coupled with monochromators for the electron beam and computational algorithms for analyzing large amounts of data, now make it possible to investigate entirely new phenomena at interfaces, such as the vibrational behavior, interface diffuseness, etc. Having such capability can require careful thought as to long-standing questions regarding how to define an interface in terms of its structure, or properties. Particular attention will be paid to describe new interesting problems that can be addressed at phase transformation interfaces given these new analytical (S)TEM capabilities.

### 20:15 Invited Grain Boundary Phase-Like Transformations

*Jian Luo<sup>1</sup>; Jian Luo<sup>1</sup>; <sup>1</sup>University of California*

A piece of ice melts at 0 °C, but a nanometer-thick surface layer of the ice can melt at tens of degrees below zero. This phenomenon, known as "premelting," was first recognized by the physicist Michael Faraday. Materials scientists have

discovered that interfaces in engineered materials can exhibit more complex phase-like behaviors at high temperatures, which can affect the fabrication and properties of a broad range of materials [1]. Specifically, grain boundaries (GBs) can be considered as 2D interfacial phases that are also called “complexions” to differentiate them from thin layers of bulk (3D) Gibbs phases [1]. They can exhibit average compositions, symmetry/structure, and properties that are distinct from any 3D phase. Moreover, they can often control the materials processing (e.g., sintering), microstructure evolution, and various mechanical (e.g., strength, creep resistance) and physical (e.g., electronic, ionic, thermal & superconductive) properties. See a recent Overview in *Acta Materialia* [1]. After discussing the general background of this emerging research field of GB phase-like transformations, this talk will review a series of our on-going studies to compute GB “phase” (complexion) diagrams as a new and generally useful materials science tool via three methods. First, we use a phenomenological thermodynamic model to construct “GB lambda diagrams” to forecast high-temperature GB disorder and related activated sintering behaviors; earlier studies have been reviewed [2] and a recent study expanded the success to a ceramic system, TiO<sub>2</sub>-CuO [3]. Second, we use an Ising-type lattice model to map out the stability of bilayer complexions [4]. Third, we utilize a hybrid Monte Carlo and molecular dynamics (hybrid MC/MD) method to conduct atomistic simulations in semi-grand canonical ensembles. In one case, a new type of first-order interfacial phase-like transformations that breaks the mirror symmetry of a symmetric tilt GB has been discovered [5]. More recent hybrid MC/MD simulations computed a GB adsorption diagram with first-order GB transformations for Au-doped Si, which is supported by our prior experiment and further verified by first-principles calculations [6]. We will also discuss our on-going effort to utilize machine learning algorithms to greatly expand our capabilities to construct “GB diagrams” beyond that can be achieved by atomistic simulations. As an example of great importance to physical metallurgy, we will further discuss how the formation of 2D interfacial phases (complexions) can influence or control mechanical properties. Specifically, recent atomic-level observations made in two classical GB

embrittlement systems, bismuth (Bi) vs. sulfur (S) doped nickel (Ni), will be reviewed and critically compared. In both cases, the adsorption (segregation) of Bi or S induces strong faceting at Ni general GBs. In contrast to traditional views, both the faceting and interfacial atomic structures are dictated by the orientation of the lower-index grain surface, instead of the misorientation between the two grains. Several differences exist between the two cases. Most notably, the general GBs in the Ni-Bi exhibit highly ordered bilayer adsorbates [7] that can even go through interfacial reconstructions [8]. In contrast, the GBs in the Ni-S are more disordered; yet coupled aberration corrected electron microscopy and semi-grand canonical ensemble atomistic simulation have discovered hidden bipolar orders at general GBs that cause brittle intergranular fractures [8]. Moreover, recent studies of 2D interfacial phases or complexions shed light on several other long-standing mysteries in materials science, including the origins and atomic-level mechanisms of solid-state activated sintering [2, 3], liquid metal embrittlement [7], including the origins and atomic-level mechanisms of solid-state activated sintering [2, 3], liquid metal embrittlement [7], and other classical materials science problems such as abnormal grain growth (see the *Acta Overview* [1] and references therein). Finally, we note that analogous 2D surface phases have also been studied and utilized to improve the performance of various materials for energy-related applications, including batteries, supercapacitors, and oxygen-ion conductors (see a most recent review/perspective article [9] and references therein for detail). References: [1] Cantwell et al., *Acta Mater.* 62: 1 (2014) [2] Luo, *J. Am. Ceram. Soc.* 95: 2358 (2012); Zhou et al., *Curr. Opin. Solid State Mater. Sci.* 20:268 (2016) [3] Nie et al., *Acta Mater.* 130: 329 (2017) [4] Zhou et al., *Scripta Mater.* 130:165 (2017) [5] Yang et al., *Phys. Rev. Lett.* 120, 085702 (2018) [6] Hu et al., *Scripta Mater.* 158:11 (2019) [7] Luo et al., *Science* 333: 1730 (2011); Yu et al., *Science* 358: 97 (2017) [8] Hu et al., *Nature Comm.* 9:2764 (2018) [9] Luo, *Energy Storage Materials* 21:50 (2019).

**20:45 Break**

**Zoom Room D**

## Phase Field Modelling II

**Zoom link: TBD**

**Chairs: TBD**

**17:15 Invited**

### Phase Field Modeling of TWIP Beta Titanium Alloys

*Benoit Appolaire<sup>1,3</sup>; Juba Hamma<sup>2</sup>; Yann Le Bouar<sup>2</sup>; Alphonse Finel<sup>2</sup>; <sup>1</sup>Université de Lorraine; <sup>2</sup>Onera-CNRS; <sup>3</sup>Université de Lorraine*

Recently, new beta-metastable TRIP/TWIP titanium alloys have been developed that exhibit improved mechanical properties, i.e. high strength and ductility, accompanied by an unprecedented strain hardening for titanium alloys at ambient temperature. These mechanical properties are attributed to complex microstructures engendered by the mechanical destabilization of the initial bcc phase during deformation. Indeed, the microstructure features numerous twins following the peculiar  $\{332\} \langle 11-3 \rangle$  twinning mode, specific to beta-titanium alloys, as well as orthorhombic  $\alpha''$ ; and simple hexagonal omega phases ensued from concomitant displacive transformations. Moreover, observations have revealed the possible activation of secondary deformation mechanisms, such as secondary twins and/or  $\alpha''$ ; inside primary twins. In view of better understand the formation of the complex microstructures described above, we have developed a phase field model focusing on the  $\{332\} \langle 11-3 \rangle$  twinning mode. Phase field models proposed so far for deformation twinning exhibit several essential flaws preventing them to be applied in our case. First, some of them formulate the elastic energy using the small strain approximation. Considering the large shear components of the eigenstrain associated with twinning ( $\sim 35\%$  for  $\{332\} \langle 11-3 \rangle$  twins), the use of the infinitesimal strain theory is not justified, in particular because the accommodation mechanism resulting from the crystalline rotations are not correctly accounted for. Second, the proposed models are all restricted to primary twinning by construction, meaning that the free energy landscape is built in such a way that it cannot allow the formation of secondary

twinning. In this work, we propose a phase-field model free of the first deficiency, relying on a finite strain formalism. We will show the capabilities of this model to simulate the formation and evolution of the complex microstructures observed in TWIP titanium alloys. In addition, a comparison with a model formulated in a small strain formalism will be presented to show the influence of the geometrical non-linearities introduced in the finite strains framework. Finally, the analysis of particular locations in the microstructure where stresses and strain are the largest will suggest a further extension of the model to handle secondary twinning.

**17:45 Invited**

### Rafting in Nickel Base Superalloys: A Phase Field Study

*Yann Le Bouar<sup>1</sup>; Maeva Cottura<sup>2</sup>; Benoit Appolaire<sup>2</sup>; Alphonse Finel<sup>1</sup>; <sup>1</sup>Universite Paris-Saclay; <sup>2</sup>Universite de Lorraine*

Mechanical properties of metallic materials strongly depend on their microstructure, i.e. on the shape and spatial arrangement of the different phases in the materials. It is thus important, from both fundamental and industrial viewpoints, to understand and control the microstructure evolution. The phase field method as emerged as the most powerful method for tackling microstructure evolutions during phase transformations, especially when elastic coherency stresses are generated in solids. However, in many materials, the microstructure evolutions are coupled with a plastic activity, and there is currently a great research effort to extend the phase field method to take this coupling into account. Within the phase field approach, plasticity can be incorporated either at the scale of dislocations or in a continuous framework. In this work, a classical phase field model is coupled to a crystal plasticity model based on dislocation densities [1]. This model includes the anisotropy as well as the size-dependence of the plastic activity, which is expected when plasticity is confined in region below few microns in size. The model uses a storage-recovery law for the dislocation density of each glide system and a hardening matrix to account for the short-range interactions between dislocations. The proposed coupled model will be applied in two and three dimensions to study the rafting of ordered

precipitates in Ni-base superalloys. Several creep conditions will be analyzed such as tensile loadings along [001], [011] and [111] directions, and the role of small misorientations around these axis will be considered. First, the plastic driving force for rafting will be analyzed using the phase field model in which plasticity is turned off. The importance of the inhomogeneity of the shear moduli  $C_{44}$  and  $C'$  will be demonstrated and rationalized using a mean field approach. Then, the plastic driving force will be considered using the full phase field model, and the evolution of the dislocation densities in the gamma channels will be analyzed. Finally, model simulations will be designed to quantitatively compare plastic and elastic driving forces. [1] M. Cottura, B. Appolaire, A. Finel, Y. Le Bouar, J. Mech. Phys. Solids, 94, 473-489, 2016.

**18:15 Break**

**Phase Field Modelling III**

**Chairs: TBD**

**19:15 Invited**

**Phase Field Modeling for Solid-state Synthesis**

*Katsuyo Thornton; University of Michigan*

Solid-state synthesis, in which a mixture of compounds is heated to induce reaction and phase transformation, is widely used to produce a wide variety of multicomponent compounds. In particular, solid-state metathesis has recently been demonstrated for synthesis of compounds that are difficult to produce by other synthesis routes. However, such a process involves at least two anion species and two cation species, leading to a highly complex thermodynamic landscape as well as kinetic limitations. Therefore, the fundamental understanding behind the metathesis reaction is lacking, and it is unclear what material properties govern the reaction products under what synthesis conditions. The phase field modeling approach is uniquely suited to elucidate such processes because it accounts for the interplay between the thermodynamics and kinetics. In this presentation, a phase field model for systems containing

ionic mixtures will be described, and the simulation results will be presented, along with the insights gained. The model is implemented into PRISMS-PF, an open-source phase field framework developed within the PRISMS Center, a DOE Software Innovation Center. This work was supported as part of GENESIS: A Next Generation Synthesis Center, an Energy Frontier Research Center funded by the U.S. DOE, Office of Science, Basic Energy Sciences under Award Number DE-SC0019212.

**19:45 Invited**

**Revisiting Heterogeneous Nucleation at Homo/Hetero-Interface**

*Rongpei Shi; Harbin Institute of Technology (Shenzhen)*

Even though theoretical models on heterogeneous nucleation (HN) at homo-phase grain boundaries (GBs) and inert substrate were established decades ago, our understanding of HN at both homo-phase and hetero-phase interfaces remains far away from being complete. By using a fully variational approach, we demonstrate for the first time that a nucleus with low-energy facet(s) is highly deformable in response to its interaction with the GB along the triple junction line. Consequently, the nucleus shape deviates significantly from the one predicted using Wulff-construction, and the energy of formation can be reduced by orders of magnitude relative to predictions by previous methods. As another example, we extend, for the first time, the classical nucleation theory to HN of a thermodynamically stable phase at hetero-phase interfaces between the original and the precursory metastable phases, which are frequently encounter in two-step nucleation pathway. Our extended model demonstrates that the nucleus shape along the minimum energy path is strongly size-dependent, and this additional degree of freedom can result in the reduction of the critical nucleus volume and associated activation energy barrier by orders of magnitude relative to conventional predictions.

**20:15 Contributed**

**Phase Field Model of L10-type Ordering Kinetics**

*Ryuichiro Oguma<sup>1</sup>; Long-Qing Chen<sup>2</sup>; Syo Matsumura<sup>3</sup>; <sup>1</sup>Fukuoka University; <sup>2</sup>The Pennsylvania State University; <sup>3</sup>Kyushu University*

A phase-field model for ordering process of L10 type in



binary alloys is formulated, taking into account the crystallographic relations between ordered and disordered states. A lattice distortion which occurs along c-axis during the ordering process is considered to investigate the effects of elastic strain energy on the domain formation process. The formation and evolution of domain structures was simulated by solving numerically the kinetic evolution equations for the order parameters and concentration. The results obtained well reproduced microstructures observed by transmission electron micrography (TEM).

**20:45 Break**

*PTM*  
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Thursday | 30 JUNE 2022 GMT+8 (Beijing)

**Zoom link: TBD**

**Chairs: TBD**

**16:00 Plenary**

### **Role of Interfaces on the Morphology of Phase Transformation Products**

*Wenzheng Zhang; Tsinghua University*

The morphologies of phases developed from solid-state phase transformations play a key role in material properties not only due to the shape of the phases, but also to the orientation relationships (ORs) of the new phases with respect to their matrix and to the nature of the interfaces surrounding the new phases. The morphologies in many materials are characterized by the interfaces with preferred geometries, including the interfacial orientations and the ORs, while random interfacial geometries are also observed in some other materials. This talk will emphasize two key features in interfaces for quantitative interpretations of preferred interfacial geometries. One key feature is the preferred state (PS) that has a strong tendency to form locally at the early stage of a phase transformation. As defined by Bollmann, a PS is a low energy matching state with either fully or coincidence-site coherent structure. Existence of a PS in an interface between the new phase and the matrix is the necessary condition for the interface to have a preferred geometry, especially the OR, while the interface may have a random geometry if a PS is developed between the new and a non-matrix phase (or grain) due to nucleation at an existing interface. Based on the periodic nature of a PS, we developed a method to predict potential PSs and the corresponding interfacial geometries for a given pair of phases. The final geometry of a preferred interface depends on the development of the interfacial dislocations, which are the other key feature in interfaces. We found that a preferred interface must contain a singular dislocation structure characterized with singularity and periodicity. The O-lattice theory has been extended to facilitate the dislocation calculation and to specify the interfacial geometries

corresponding to singular dislocation structures. Accordingly, we proposed a set of general rules for identifying discrete geometries of preferred interfaces and applied successfully to the interpretations of preferred interfaces observed in different materials. However, prediction of final preferred geometries of interfaces in a given system remains an unreached goal, except for simple cases with negligible misfit from an obvious PS. The final result depends on generation of the above two key features during a phase transformation, but the knowledge about this process is rather limited. A discussion will be made on the generation of these key features, to link thermodynamics and kinetics with crystallography of a transformation. This discussion may shed some light on the influence of the transformation conditions on the morphology of the new phases and stimulate further investigations.

**17:00 Break**

**21:15 Award ceremony**

**Zoom Room A**

### **Precipitation in Steels**

**Zoom link: TBD**

**Chairs: TBD**

**17:15 Contributed  
 Vanadiumcarbide interphase precipitation  
 studied in-situ by neutron scattering**

*Sven Erik Offerman<sup>1</sup>; Chrysoula Ioannidou<sup>1</sup>; Alfonso Navarro-López<sup>1</sup>; Ad van Well<sup>2</sup>; Jilt Sietsma<sup>1</sup>; Catherine Pappas<sup>2</sup>; Arjan Rijkenberg<sup>3</sup>; Robert Dalgliesh<sup>4</sup>; <sup>1</sup>Delft University of Technology; <sup>2</sup>Delft University of Technology; <sup>3</sup>Tata Steel; <sup>4</sup>Rutherford Appleton Laboratory*

We study the interaction between vanadiumcarbide precipitation and phase transformation kinetics simultaneously by means of in-situ neutron scattering. We developed a furnace for in-situ studies of interphase precipitation in steel by means of simultaneous small-angle neutron scattering and neutron diffraction to study precipitation and phase transformation kinetics, respectively. Steels with three different vanadium and carbon concentrations are studied at two different temperatures of 650 and 700°C. Increased amounts of vanadium and carbon to the steel composition cause a retardation of the phase transformation kinetics. The effect of each alloying element on the observed phase transformation kinetics can be described by its contribution to the Gibbs free energy dissipation related to solute drag. The vanadiumcarbide precipitation is initiated by the austenite-to-ferrite phase transformation. Larger and fewer precipitates are observed at 700 than at 650 °C in the three steels. A larger number density of precipitates is detected in the steel with higher concentrations of vanadium and carbon. We observe composition changes in the vanadiumcarbide precipitates during annealing. The external magnetic field applied during the experiments, necessary for the SANS measurements, causes a delay in the onset and time evolution of the austenite-to-ferrite phase transformation and consequently on the precipitation kinetics.

### 17:30 Contributed

#### Modeling Approach to the Solubility Product of TiN in Austenite by Measuring the Grain Growth

*Wei Wang<sup>1</sup>; <sup>1</sup>Baosteel Research Institute*

Titanium (Ti) is nearly the mostly used microalloying (MA-ing) element, not only because that it is the cheapest among the MA-ing elements, but also that it plays an important role in both precipitation strengthening and grain size control, especially at high temperature. Titanium nitride (TiN) is the first to form in austenite even just after steel making and its volume and size influence the subsequent precipitation, microstructure evolution and the final properties. It is hence important to precisely model the precipitation of TiN during both heat up and cooling process, and a good solubility product (SP) of TiN is a key to achieve this. Many SP equations of TiN have been obtained by different methods

and also, maybe, for different alloying systems. As the result of this, the calculation by those equations falls in a large range. It is therefore essential to assess the equations and find a right one for each steel system.

In this paper, SP equations of TiN in austenite are briefly reviewed. Then followed by a modeling analysis on the austenite grain growth with considering the pinning effect, and the Ostwald ripening of TiN particles. The models are simultaneously evaluated with a series of austenite grain sizes obtained by designed experiment with a plain carbon steel. An SP equation is thereafter obtained and compared with those in literature.

### 17:45 Contributed

#### Interphase Precipitation of Nano-sized Alloy Carbide in V-Nb and V-Ti Multiple Microalloyed Low-carbon Steels

*Yongjie Zhang<sup>1</sup>; Goro Miyamoto<sup>1</sup>; Tadashi Furuhashi<sup>1</sup>; <sup>1</sup>Tohoku University*

Ferritic steels strengthened by interphase precipitation of nano-sized alloy carbide formed during austenite-to-ferrite transformation by have been widely used in industry for its high strength with excellent formability. In this study, interphase precipitation behaviors in V-Ti and V-Nb microalloyed low-carbon steels were systematically investigated, for a better understanding of its nature in multiple added alloy systems. A series of Fe-0.1C-1.5Mn-0.05Si (mass%)-based alloys with 0.1V-0.1Nb and 0.1V-0.05/0.1Ti multiple additions were mainly used, with their corresponding single additions as well for comparison. After austenitization, all the alloys were isothermally transformed at 963K and 923K for various times, followed by water quenching. Afterwards, the details of alloy carbide in terms of both chemical composition and dispersion were quantitatively analyzed by using three-dimensional atom probe (3DAP), while the hardness of ferrite was measured to evaluate the precipitation strengthening. The experimental results revealed that regardless of the transformation temperature, V, Nb and Ti atoms are homogeneously distributed in interphase precipitated nano-sized alloy carbide, without forming any core-shell structure. In addition, comparatively stronger enrichment tendency into

alloy carbide of Nb and Ti than V, especially at the early stage of ferrite transformation, was clearly identified. When compared with the same total addition of carbide-forming elements, the multiple added alloys represented a moderate number density and average radius of alloy carbide falling between the trends of single added cases, resulting in medium amounts of strengthening.

**18:15 Break**

## Precipitation in Steels

**Chairs: TBD**

**19:15 Contributed**

### A Study on the Alloying Strategy to Tune Carbide Precipitation in a High-performance Cr-Mo-V-alloyed Steel

*Tao Zhou<sup>1</sup>; R. Prasath Babu<sup>1</sup>; Joakim Odqvist<sup>1</sup>; Peter Hedström<sup>1</sup>; Tao Zhou<sup>1</sup>; <sup>1</sup>KTH Royal Institute of Technology*

Carbide precipitation is widely used to improve the properties and performance of tool steels. Aiming at tailoring the carbide precipitation to achieve the optimum performance, this work studies multiple carbide precipitation during isothermal tempering of a low-alloy Cr-Mo-V steel. Quantitative information of carbide precipitation from transmission electron microscopy (TEM) is used to compare with/calibrate the physically based modelling by mean-field numerical-Kampmann-Wagner (NKW) approach making use of CALPHAD-type databases. Yield strength is further modelled by semi-empirical models with input from the calibrated NKW modeling and characterization of other microstructural features. The predicted strength is compared with data from tensile testing. In addition, thermodynamic calculations is used to suggest further improvements to stimulate precipitation of fine carbides (MC and M2C) by tuning alloying and heat treatments. The methodologies presented in this work, i.e. the combination of quantitative characterization, NKW modelling of precipitation, thermodynamic calculations as

well as semi-empirical modelling of the strength are promising for optimization and design of high-performance tool steels.

**19:30 Contributed**

### On The Origin of Non-Cube-on-Cube Orientation Relationship Between M23C6 and Austenite in An Austenitic Stainless Steel

*Guanghui Chen<sup>1,3</sup>; Reza Rahimi<sup>2</sup>; Horst Biermann<sup>2</sup>; Javad Mola<sup>1</sup>; <sup>1</sup>Osnabrück University of Applied Sciences; <sup>2</sup>Technische Universität Bergakademie Freiberg; <sup>3</sup>Wuhan University of Science and Technology*

The type, stability temperature range, and crystallographic orientation relationship of chromium-rich carbides with the austenitic matrix of a novel Al-added stainless steel with the chemical composition Fe-17Cr-9Ni-6Mn-4Al-0.4C (wt.%) was investigated by differential scanning calorimetry (DSC), metallography, and diffraction analyses in scanning electron microscope (SEM) and transmission electron microscope (TEM). DSC measurements indicated two endothermic peaks associated with the dissolution of two types of carbides. Electron backscatter diffraction (EBSD) analysis of the steel after homogenization annealing at 1200 °C and cooling at an average cooling rate in the temperature range 1200-600 °C of 2.5 °C indicated the coexistence of coarse M7C3 carbides and a finer array of M23C6 carbides, with M primarily representing Cr and Fe. The approximate position of poles in the pole figures for the M23C6 carbides with the space group (face-centered cubic structure with  $a \approx 1.06$  nm) resembled those for the body-centered cubic lath martensite formed while maintaining Kurdjumov-Sachs (K-S) orientation relationship with the austenitic matrix. The multiplicity of crystallographic variants of M23C6 carbides in the austenite is in sharp contrast with the existing reports that such carbides maintain a cube-on-cube orientation relationship ( , ) with the austenitic matrix and that the number of crystallographic variants might only increase to a total of five by twinning. Aging of the homogenized steel at 800 °C resulted in the formation of a large volume fraction of fine M23C6 carbide platelets in the austenitic matrix. The fine size of the newly-formed carbide platelets precluded their characterization by EBSD. Selected area electron diffraction (SAED) analysis of M23C6



platelets in TEM indicated that in contrast to the M23C6 carbides in the as-homogenized condition, the carbide platelets formed in the austenite during aging at 800 °C had a cube-on-cube or twin orientation relationship with the austenite. The large number of M23C6 variants with non-cube-on-cube orientation relationship in the as-homogenized condition was explained by their formation via intermediate M7C3 phase. The M23C6 carbide platelets formed during aging at 800 °C, on the other hand, formed by direct nucleation in the austenite and their orientation relationship was hence compatible with the existing reports. Keywords: M23C6; M7C3; carbides; transformation; austenitic stainless steel; crystallographic orientation relationship

### 19:45 Contributed In Situ Characterization of Phase Transformations in A JIS G3106 SM490A-FR Fire Resistant Steel, during Fire Simulations

*Andre Tschiptschin<sup>1</sup>; Julian David Escobar<sup>1,2</sup>; Filipe Moreno Carvalho<sup>3</sup>; Pedro Meirelles Gomes<sup>1</sup>; Hélio Goldenstein<sup>1</sup>; <sup>1</sup>University of S&#227; <sup>2</sup>Pacific Northwest National Laboratory; <sup>3</sup>Sao Paulo State Technological Research Institute*

Fire-resistant steels (FRS) are high strength low alloy steels modified by micro-alloying of carbonitride forming elements, such as Ti, V and Nb. This promotes the formation of beneficial nanosized MCN-type secondary precipitates. Besides, the addition of substitutional elements, such as Ni, Cr and Mo has been used to retard the thermally-activated microstructural decomposition during the exposure to fire. In this work, a commercial Fe-0.1C-1Mn-0.4Mo-0.03V FRS was used in order to study the decomposition kinetics of different initial microstructures, such as ferrite-pearlite, bainite and martensite. In situ observations were performed by high energy synchrotron X-ray diffraction in transmission mode during the simulation of a fire cycle, using a Bähr DIL 805 dilatometer at the P07 beamline at the Deutsche Synchrotron DESY. The in situ observation of the secondary precipitation of cementite was possible through a carefully designed peak isolation and normalization methodology, sensitive to very small changes in intensities. Firstly, the diffraction spectra were trimmed in order to isolate a 2q

range containing a large number of cementite peaks with no presence of volumetric phases. Then, both the background and peak intensities were adjusted by a second-grade equation describing the evolution of intensity as a function of temperature. A reference artificial peak was calculated and its evolution was used to normalize the real cementite peaks. This allowed subtracting the contribution of temperature to the increase in intensity during the heating stage. The as-received hot rolled ferritic-pearlitic microstructure showed very little secondary precipitation, only above 500 °C. The bainitic and martensitic microstructures showed little or no initial cementite presence. However, upon heating, strong secondary precipitation occurred at 410 and 350 °C, for the bainitic and martensitic microstructures, respectively. The latter evidenced incomplete precipitation upon heating but reached completion after 60 seconds of isothermal exposure at 600 °C. Cementite precipitation occurred via carbon partition from the super-saturated matrix and retained austenite. Although the steel presented high temperature strength compatible with fire resistant steels, vanadium carbonitrides were not detected, suggesting that Mo is the key alloy element granting fire resistance properties.

### 20:00 Contributed A Simplified Growth Model for Multicomponent Precipitation and Its Implementation in TC-PRISMA

*Qing Chen<sup>1</sup>; Kaisheng Wu<sup>1</sup>; Johan Jeppsson<sup>1</sup>; John Ågren<sup>1</sup>; <sup>1</sup>KTH Royal Institute of Technology*

A general simplified model for the growth of particles in a multicomponent system has been developed. The model takes into account of the effects of cross diffusion, high-supersaturation, and finite interface mobility. It can be applied in a straightforward way to treat precipitation under the condition of para-equilibrium (PE) or non-partitioning local equilibrium (NPLE) without resorting to a usually difficult and time-consuming solution of the coupled flux balance and local equilibrium equations under the influence of the Gibbs-Thomson effect. The model has been implemented in TC-PRISMA, a computational tool to treat concurrent nucleation, growth, and coarsening of multiple phase precipitates in multicomponent alloy systems. TC-

PRISMA is available as a module in the Thermo-Calc Software package and has direct access to thermodynamic and kinetic databases developed for various kinds of alloys over decades. The proposed model has been applied to simulate the precipitation of carbides during tempering of steels. A few case studies will be shown and discussed. Partial support from VINNOVA, the Swedish Governmental Agency for innovation Systems and Swedish industry, is acknowledged.

**20:15 Break**

**Interdiscipline I**

**Chairs: TBD**

**20:30 Invited**

**Mobilities of Coherent and Incoherent Interfaces in the Au-Fe Nanowhiskers**

*Eugen Rabkin<sup>1</sup>; Yuanshen Qi<sup>1</sup>; Gunther Richter<sup>2</sup>; Leonid Klinger<sup>1</sup>; <sup>1</sup>Technion; <sup>2</sup>Max Planck Institute for Intelligent Systems*

We conducted a series of systematic diffusion measurements on Au-Fe bimetallic nanowhiskers. Defect-free <110>-oriented Au nanowhiskers having {001} and {111} side facets were grown by molecular beam epitaxy technique, followed by another deposition of Fe layers. The Fe layers deposited on {001} and {111} Au facets were single- and polycrystalline, respectively. Focused ion beam (FIB) milling and lift-out technique were used to harvest individual Au-Fe nanowhiskers for heat treatments and subsequent transmission electron microscopy (TEM) samples (nanowhisker cross-section) preparation. Scanning transmission electron microscopy (STEM) with atomic resolution high-angle angular dark-field (HAADF) imaging and electron energy loss spectroscopy (EELS) scanning were carried out for the characterization of the atomic structure of interfaces and composition distribution in their vicinity. We uncovered anisotropic penetration of Fe in Au along <001> and <111> directions, even though the diffusion in cubic crystal should be isotropic. The penetration depth of Fe in Au along <001> was much shorter

than it was along <111> direction and both were shorter than the values estimated from the literature data on bulk diffusion of Fe in Au. We attributed this anisotropic intermixing to the difference in mobility of different Fe-Au interfaces. We developed a kinetic model allowing quantitative determination of interface mobilities from our interdiffusion data. The slow mobility of the coherent Fe-{001} Au interface was correlated with its atomic structure. We demonstrated that the coherent interface moves by migration of the interface disconnections.

**21:00 Contributed**

**Phase Transformations during Nitriding of Microstructurally and Compositionally Heterogeneous Fe-C-Si Alloys – Nitriding of White-solidified Cast Irons**

*Stefan Kante<sup>1</sup>; <sup>1</sup>TU Bergakademie Freiberg*

Nitriding of white-solidified Fe-C-Si cast irons results in complex microstructures due to the heterogeneity of the substrate material. The growth rate and the phase composition of the compound layer vary spatially and temporally among Si-rich, C-poor pearlitic regions and Si-free, C-rich eutectic cementite. The precipitation of amorphous Fe-containing Si nitride plays a crucial role to the microstructure evolution. The latter involves two isothermal, chemical potential-driven eutectoid transformations, upon which amorphous Si nitride forms cooperatively with a crystalline matrix phase, i.e. α-Fe or ε-(carbo)nitride.

**Zoom Room B**

**Advanced High Strength Steels**

**Zoom link: TBD**

**Chairs: TBD**

**17:15 Invited**

### Carbon Enrichment at Coating/substrate Interface and its Effect on Bendability of Al-Si Coated Press Hardening Steel

Hongliang Yi<sup>1</sup>; L. L. Zeng<sup>1</sup>; D. P. Yang<sup>1</sup>; S. Zhou<sup>2</sup>;  
<sup>1</sup>Northeastern University; <sup>2</sup>Easyforming Materials Technology Co., Ltd.

Al-Si coated press hardening steel (PHS) is widely applied on carbody due to its high strength exceeding 1500MPa. However, the Al-Si coating was found to seriously deteriorate the fracture strain. In this research, the fracture process of a press-hardened Al-Si coated PHS during bending test was investigated. The Al-enriched alloying layers involving the intermetallic layers and the ferrite layer are not able to inhibit the crack propagation, but the cracks are then blunted by the hard martensite substrate. Finally, fracture happens by the shear band initiation and propagation from the surface of martensite. The carbon enrichment about several micrometers in martensite at the coating/substrate interface after press-hardening was found for the first time to deteriorate the bending fracture strain of Al-Si coated PHS. A novel method of reducing the coating thickness was then invented to suppress the carbon enrichment by suppressing the coating/substrate interface migration. This leads to improve the fracture strain ~20% and the strength ~5% simultaneously.

### 17:45 Contributed

#### Engineering the High-Mn TRIP Steel via Heavy Ausforming

Qingquan Lai<sup>1</sup>; Qi Lu<sup>2</sup>; Hao Zhou<sup>1</sup>; Thomas Pardoen<sup>3</sup>;  
<sup>1</sup>Nanjing University of Science and Technology; <sup>2</sup>General Motors Global Research and Development; <sup>3</sup>Universite catholique de Louvain

This study explores the effect of heavy ausforming on the microstructure and mechanical properties of a high-Mn steel. The coarse-grained microstructure consisting of 87vol.% of epsilon-martensite presents limited mechanical properties as well as a brittle fracture behavior. By means of heavy ausforming with 90% rolling reduction, an ultrafine-grained microstructure is produced, associating with the significant increase of the austenite volume fraction. Under mechanical loading, the austenite is gradually transformed into epsilon-martensite, and the transformation-induced plasticity leads

to a surprisingly high combination of strength, uniform elongation and fracture strain. A ductile fracture mode with improved resistance to damage initiation in the ultrafine-grained microstructure contrasts with the brittleness of the coarse-grained counterpart. The impressive mechanical performance of the heavily-ausformed microstructure is attributed to the formation of ultrafine-grained epsilon-martensite, in which non-basal <c+a> slips are dominant in the plastic deformation instead of mechanical twinning. This finding inspires the development of high-performance metastable alloys with economical composition relying on engineering the prior austenitic microstructure.

### 18:00 Contributed

#### Effect of Si on Microstructure and Mechanical Properties of FeMnAlC Lightweight Steels

Zhangwei Wang<sup>1</sup>; <sup>1</sup>Central South University

We systematically investigated the influence of Si on the microstructural evolution and mechanical properties of Fe-30Mn-9Al-1.2C-xSi (x=0, 1, 2 wt. %) lightweight steels under the as-homogenized state. By employing the most state-of-the-art characterization techniques, e.g., aberration-corrected transmission electron microscopy (TEM) and atom probe tomography (APT), the dislocation substructure and phase evolution in the steels were revealed at atomic scales. With the increase of Si content from 0 to 2 wt. %, the average sizes of  $\epsilon$ -carbides in the austenite matrix increase from ~1 nm to ~12 nm. In addition, particle-shaped  $\epsilon$ -carbide and  $\delta$ -ferrite are formed at grain boundaries in the steel with 2 wt. % Si. The growth of  $\epsilon$ -carbide in grain interior further causes a strong precipitate strengthening effect, leading to the increase of yield strength from ~450 MPa to ~900 MPa as the Si content increases from 0 to 2 wt. %. The primary deformation mechanism is the formation of slip bands in all the three steels, which involves the shear of  $\epsilon$ -carbides upon straining. The present study provides valuable insights into the design of lightweight steels with higher specific strength via the addition of lightweight elements.

### 18:15 Break

## Advanced High Strength Steels

Chairs: TBD

### 19:15 Contributed

#### On the Significance of Austenite Stability and Microstructural Morphology on the Mechanical Properties and Work Hardening Behaviors of Medium Mn Steels

*Yu Zhang<sup>1</sup>; Hua Ding<sup>1</sup>; <sup>1</sup>Northeastern University*

One interesting characteristic in tensile behaviors of medium Mn steels is fairly long Lüders band governed yield point elongation. However, no Lüders band governed elongation but better work hardening was observed in the engineering stress-strain curves of medium Mn steels with lath-typed microstructure. Previous researches have suggested that Lüders band governed elongation in medium Mn steel could be ascribed to the interaction between mobile dislocations and the interstitial atoms, namely Cottrell atmosphere. In the present study, we proposed a novel explanation to expatiate the essence of Lüders band governed elongation in ultrafine-grained (UFG) medium Mn steels and further elucidate the reason for the better work hardening ability in medium Mn steels with lath-typed microstructure. Intercritical annealing (IA) and austenite reversed transformation (ART) were adopted to obtain granular and lath-typed UFG ferrite/austenite dual phase microstructure in cold rolled medium Mn steels, respectively. A long yield point elongation was observed in engineering stress-strain curve of IA sample and XRD analysis showed that significant TRIP effect occurred in IA sample. Based on the surface observation of IA sample during tensile test, the unique behavior of Lüders band propagation could be attributed to the inhomogeneous deformation caused by the counteraction between strain softening of UFG-scaled microstructure and strain hardening induced by TRIP effect. It should be noted that in ART sample, the width of lath was in UFG scale, while the length of lath was in micrometer scale. It was the micrometer-scaled length of lath that accommodated the generation and accumulation of dislocations, leading to an

improvement in work hardening ability. It was of great significance that mechanical properties and work hardening behavior of medium Mn steels could be modified by tailoring the austenite stability and microstructural morphology.

### 19:30 Contributed

#### The Mechanism of Mn Partitioning in Medium Mn Steels

*Qinyi Guo<sup>1</sup>; Haiwen Luo<sup>1</sup>; <sup>1</sup>University of Science and Technology Beijing*

Although the partitioning of Mn during ferrite-to-austenite transformation plays a critical role in the formation of sufficient austenite for achieving the excellent mechanical properties of medium Mn steels, why substitutional Mn atoms can be rapidly partitioned to near-equilibrium content remains mysterious. We investigated this mechanism by both the experimental measurement at the atomic scale and the kinetic modeling. Numerous simulations were conducted with a variety of assumptions both for the diffusivity of Mn in austenite and martensite/ferrite and for the interface mobility. Compared to the diffusion-controlled transformation kinetics, the assumed interface mobility term reduced the interface migration rate, resulting in much higher values of the interfacial Mn concentration. In addition, fluctuating interface mobility was proposed since it can best fit the Mn and C concentration gradients near the interface measured by atomic probe tomography, and the microstructural processes that lead to the Mn compositional fluctuations in austenite were also discussed in this study.

### 19:45 Contributed

#### Architecturing Medium Mn Steels with Novel Microstructure and Mechanical Properties

*Ran Ding<sup>1</sup>; Yingjie Yao<sup>1</sup>; Geng Liu<sup>1</sup>; Binhan Sun<sup>2</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>Tsinghua University; <sup>2</sup>Max-Planck-Institut für Eisenforschung GmbH*

Improving the mechanical performance of structural materials is vital to our society. To achieve this goal, tuning phase transformation behaviors to realize suitable microstructure is one of the most effective routines. Here, a new dimension of microstructural design is proposed. Massive nano-scaled chemical heterogeneities are created



by the ultrafast heating technology. As a result, the martensitic transformation is restricted within very fine domains, leading to a novel ultrafine martensite + austenite duplex microstructure in a medium Mn steel. The mechanical properties are unprecedentedly improved as compare with those after conventional intercritical annealing treatments. Without high carbon content and/or doping expensive elements which are frequently used to guarantee a high strength, the ultimate tensile strengths achieved by this new method are in excess of 2.0 GPa in combination with high ductility. The mechanisms of microstructural evolution and deformation behaviors are investigated in the present study. Additionally, this methodology in principle can be applied to other alloy systems.

**20:00 Contributed**

**Homogeneous Elasto-Plastic Deformation and Improved Strain Compatibility between Austenite and Ferrite in a Co-precipitation Hardened Medium Mn steel with Enhanced Hydrogen Embrittlement Resistance**

*Yu Li<sup>1</sup>; Wei Li<sup>2</sup>; Xuejun Jin<sup>2</sup>; <sup>1</sup>Shanghai Institute of Technology; <sup>2</sup>Shanghai Jiao Tong University*

A co-precipitation hardened medium-Mn steel with respective NiAl and Cu-rich particles in dual phases (austenite and ferrite) has been designed by a quenching-partitioning-tempering (QPT) treatment. Compared to the Cu-Free steel, in which single NiAl precipitates form in ferrite, co-precipitation in the Cu-Added steel results in an improved strain compatibility between austenite ( $\gamma$ ) and ferrite ( $\alpha$ ). Lattice strains of both  $\gamma$  and  $\alpha$  phases show similar evolutions during the entire strain regime, and homogeneous elasto-plastic deformation occurs together with a continuous yielding and weak transient of strain hardening rate. The improved strain compatibility leads to alleviation of strain localization in the phase interfaces, so that the overall back stress increases slowly with the tensile strain increasing during the whole plastic deformation process, although both medium Mn steels possess similar tensile strength (1 GPa) and elongation (25%) values.

**20:15 Break**

**Industrial Applications**

**Chairs: TBD**

**20:30 Invited**

**Exploring High Carbon Bearing Steels with Silicon Additions**

*Hélio Goldenstein<sup>1</sup>; <sup>1</sup>Escola Politécnica da Universidade de São Paulo*

Hypereutectoid steels containing 1% C and 1.5% Cr, intercritical annealed so as to obtain a distribution of spheroidized carbides on a tempered martensite matrix, have been used for bearings and other machine components subjected to rolling and contact fatigue, for more than a century. This work describes a series of researches conducted in our group over the last decade involving the study of Fe-C-Mn-Si-Cr alloys similar to AISI 52100 or DIN 100Cr6, modified with added silicon on the order of 1.8%. Initially the modified steels were designed to delay the cementite precipitation kinetics and thus prevent or delay the occurrence of tempered martensite brittleness (TMB) and increase the softening resistance, allowing for tempering at higher temperatures and thus leading to new processing routes, mimicking the alloy design of 300M steels on behalf of AISI 4340. Shortly afterwards, after taking notice of the similarity of those steels with the alloys used by the Cambridge group for obtaining the nanobainite structure, we explored the idea of obtaining a nanobainitic matrix, while keeping the distribution of spheroidized carbides obtained by an intercritical austenitization. Other groups explored similar routes, establishing that the key for improved fatigue resistance involves obtaining stable retained austenite, as structures containing metastable retained austenite did not fare well on cyclic mechanical tests. More recently our group is exploring the possibilities of the quenching and partition (Q&P) heat treatment as a means to obtain a structure containing a fine distribution of carbides within a complex phase matrix, containing low temperature tempered martensite, stable austenite films and carbide free bainite. This research is being conducted using dilatometry and in-situ synchrotron XRD studies and is an ongoing project.

**21:00 Contributed**

**Characterization of Microstructure Transformed from Pancaked Austenite Grains in a Large-thickness X80 Pipeline Strip Steel**

*Qingyun Sha<sup>1</sup>; <sup>1</sup>ANSTEEL GROUP CORPORATION LIMITED*

Characterization of microstructure transformed from pancaked austenite grains in an industrial hot-rolled X80 pipeline strip steel with the thickness of 18.4mm has been investigated using optical microscopy (OM), scanning electronic microscopy (SEM) and transmission electronic microscopy(TEM). The X80 strip steel was etched with an improved etchant. Both the pancaked austenite grain boundaries (AGB), and acicular ferrite (AF), granular bainite (GB), banitic ferrite (BF) inside pancaked austenite grains are clearly revealed. The revelation of pancaked AGB indicated the higher cooling rate after finish rolling and excellent hardenability of large-thickness X80 strip steel. This is also confirmed by the estimated cooling rate during continuous cooling process and measured CCT curve for X80 steel in this study. It is found that the size of transformed microstructure inside the austenite grains become finer with decreasing the distance of short axis of pancaked austenite grains. The distance of short axis of pancaked austenite grain is closely related to yield strength and drop weight tear test (DWTT) results (low temperature toughness) of X80 steel. OM and SEM observation show that AF forms mainly within austenite grains and GB nucleates at AGB and grows into austenite grain. In case of BF, it forms at AGB and penetrates into austenite grain. M/A constituents are found to be formed both inside austenite grain and on AGB. TEM observation reveals that microstructure contains high density dislocation. Grain refinement strengthening and dislocation strengthening are the main mechanisms operating in X80 strip steel, which contribute to the high strength and excellent toughness in this work.

Zoom Room C

**High-entropy Alloy and Ni-superalloy**

**Zoom link: TBD**

**Chairs: TBD**

**17:15 Invited**

**Ultrahigh-Strength and Ductile Alloys with Coherent Nano-Lamellar Architectures** *Zengbao Jiao<sup>1</sup>; <sup>1</sup>Hong Kong Polytechnic University*

Nano-lamellar materials with ultrahigh strengths and unusual physical properties are of technological importance for structural applications. However, these materials generally suffer from low tensile ductility, which severely limits their practical utility. In this talk, we show that markedly enhanced tensile ductility can be achieved in coherent nano-lamellar high-entropy alloys, which exhibit an unprecedented combination of over 2 GPa yield strength and 16% uniform tensile ductility. The ultrahigh strength originates mainly from the lamellar boundary strengthening, whereas the large ductility correlates to a progressive work-hardening mechanism regulated by the unique nano-lamellar architecture. The coherent lamellar boundaries facilitate the dislocation transmission, which eliminates the stress concentrations at the boundaries. Meanwhile, deformation-induced hierarchical stacking-fault networks and associated high-density Lomer-Cottrell locks enhance the work hardening response, leading to unusually large tensile ductilities. The coherent nano-lamellar strategy can potentially be applied to other alloys and open new avenues for designing ultrastrong-yet-ductile materials for technological applications.

**17:45 Contributed**

**Unveiling the Electronic Origin for the Pressure-induced Phase Transitions in High Entropy Alloys**

*Weihong Liu<sup>1,2</sup>; C.T. Liu<sup>2</sup>; <sup>1</sup>Harbin Institute of Technology (ShenZhen) ; <sup>2</sup>City University of Hong Kong*  
 Understanding and controlling pressure-related structural transformations, that can be utilized to tune functional and mechanical properties of materials, is one of the most important research themes in the materials science. However, the underlying mechanism governing the pressure-driven phase transformations in high entropy

alloys (HEAs) remains poorly understood at the present time. By combining an in-situ high-energy X-ray diffraction (XRD) technique and ab initio calculations, here we reveal the face-center-cubic (fcc) phase, rather than the hexagonal-close-packed (hcp) phase, is thermodynamically stable in the Mo<sub>x</sub>CrFeCoNi HEA system at room temperature and atmospheric pressure. However, a fcc-to-hcp transformation was identified under pressures at room temperature, resulting from a pressure-induced electronic redistribution. Remarkably, the valence electron concentration has been further demonstrated as a critical factor for regulating this pressure-related transformation, the reduction of which by Mo doping can encourage the hcp-transformation. Our studies provide new insights into the physical processes underlying the allotropic transformation that enables the feasibility of the customized alloy design of high-performance HEAs.

**18:00 Contributed**

**Evaluating Magnetic Properties of Composites from Model Alloys –application to Alternative Binder Cemented Carbides**

*ZiYong Hou<sup>1</sup>; <sup>1</sup>KTH Royal Institute of Technology*

Due to the renewed interest in alternative binders for cemented carbides it is important to understand how the binder composition influences not only mechanical properties but also the microstructure and related measurements for quality control. Microstructure and chemical composition of WC-Co is often evaluated by magnetic measurements. However, when the binder composition deviates significantly from conventional Co-based binders it is not evident that the standard measurements can be used to evaluate the same parameters. The magnetic properties of 85Ni-15Fe model alloys containing Co, W and C have been studied with the intent to isolate the influence of alloy chemistry on quality control measurements of alternative binder cemented carbides. The results show a strong influence of dissolved W on the Curie temperature and the saturation magnetization. The amount of dissolved C, and the presence of WC precipitates, on the other hand, is shown to have negligible effect. Furthermore, the magnetic coercivity is indicated to be entirely dominated

by the microstructural features and quite insensitive to composition.

**18:15 Break**

**Shape Memory Alloy**

**Chairs: TBD**

**19:15 Invited**

**Giant Elastocaloric Effect with Wide Temperature Window in Nanocrystalline Ti-44Ni-5Cu-1Al Shape Memory Alloy**

*Fei Xiao<sup>1</sup>; Xuejun Jin<sup>1</sup>; <sup>1</sup>Shanghai Jiao Tong University*

Relatively low energy efficiency and emission of refrigerant which is harmful to the environment are the two issues inevitable for the most commonly used vapor-compression refrigeration technology. Elastocaloric effect (eCE) is a possible alternative technology because some alloys show large isothermal entropy change ( $\Delta S_{iso}$ ) and adiabatic temperature change ( $\Delta T_{adi}$ ) through stress application or removal. Ti-Ni alloys are most promising eCE materials due to their large cooling ability and good workability. However, the fatigue behavior of Ti-Ni alloys must be improved. Here, we report that stable and giant eCE is obtained in nanocrystalline Ti-44Ni-5Cu-1Al (at%) alloy, which shows successive B2-B19-B19' martensitic transformation. A comprehensive study on phase transformation, microstructure, in-situ structural evolution and mechanical behavior elastocaloric effect of this alloy was studied. The maximum adiabatic temperature decrease by stress removal from 600 MPa is  $\Delta T_{adi} \sim 25$  K with a small temperature distribution of  $\sim 0.5$  K. The value of  $\Delta T_{adi}$  is consistent with that calculated from strain-temperature relation. The effective working temperature window is  $\sim 55$  K, resulting in a high refrigeration capacity of  $RC = 4.2$  kJ/kg. Material coefficient of performance reaches  $COP \sim 9.6$  when an Otto cycle is considered. The middle eigenvalue of the transformation matrix is  $\lambda_2 \sim 0.99$ , implying high lattice compatibility between the parent and martensite phases. These properties are related to diffuse nature of

successive B2-B19-B19' martensitic transformation of this alloy.

#### 19:45 Contributed

### Enhanced Elastocaloric Effect in Gradient Nanograined NiTi Shape Memory Alloy

*Junyu Chen<sup>1</sup>; Gang Fang<sup>1</sup>; Junyu Chen<sup>1</sup>; <sup>1</sup>Tsinghua University*

Motivated by the severe environmental impact of the conventional vapor-compression refrigeration technique, we fabricate an efficient and eco-friendly elastocaloric material for solid-state cooling. The coefficient of performance of material (COP<sub>mat</sub>) is a key indicator for refrigerants, but it is degenerated by material hysteresis related to the dissipative non-equilibrium aspect during phase transformation. A low-hysteresis NiTi with gradient nanograined (GNG) structures is fabricated by localized laser surface annealing on a severely cold-rolled substrate. COP<sub>mat</sub> of the GNG NiTi is enhanced by 83% while preserving a comparable adiabatic temperature change compared with that of the conventional commercial coarse-grained (CG) NiTi. Moreover, the lower operational temperature limit is extended from above 283 K to 243 K. The findings are attributed to the large specific elastocaloric ability (~4.5 K/1%) and the small stress hysteresis (~60 MPa) as a result of the gradient structure effect. The work proposes a promising strategy for optimization of thermomechanical performances of elastocaloric materials and demonstrates a great industrial potential of the GNG NiTi in solid-state cooling.

#### 20:00 Contributed

### Fatigue-resistant low-stiffness Heterogeneous Gradient Nanocrystalline NiTi Shape Memory Alloy Fabricated by Pre-Strain Laser Shock Peening

*Kai Yan<sup>1,2\*</sup>; Pengbo Wei<sup>1,2</sup>; Kangjie Chu<sup>2</sup>; Hao Wang<sup>4</sup>; Weifeng He<sup>5,6</sup>; Fuzeng Ren<sup>1</sup>; Qingping Sun<sup>2,3</sup>; <sup>1</sup>Southern University of Science and Technology; <sup>2</sup>The Hong Kong University of Science and Technology; <sup>3</sup>HKUST Shenzhen-Hong Kong Collaborative Innovation Research Institute; <sup>4</sup>Ruhr-Universität Bochum; <sup>5</sup>Xi'an Jiaotong University; <sup>6</sup>Air Force Engineering University*

The poor tensile and bending fatigue life and high stiffness have been significant obstacles in the application of NiTi shape memory alloy (SMA). Pre-strain laser shock peening (LSP) was introduced to solve these challenges. Different heterogeneous nanostructured (containing B2, B19' phase, and precipitates including Ni<sub>3</sub>Ti, Ni<sub>4</sub>Ti<sub>3</sub>) gradient residual stress layers were created by controlling the pre-strain during LSP treatment. The LSP-treated residual stress field has a two-dimensional distribution. There is compressive residual stress along the pre-strain direction at the surface region, and the maximum value increases with the pre-strain. A four-point bending fatigue test found the tension-compression asymmetry of the temperature oscillation. The stiffness decreases with pre-strain increases, while the displacement-controlled bending fatigue life improves with pre-strain increases during LSP treatment. The highest fatigue life under the maximum tensile strain of 2.4% reaches over 34000 cycles, 33 times the untreated sample, which is attributed to the surface heterogeneous nanostructure and large surface compressive residual stress. The proposed pre-strain LSP method provides a new avenue to fabricate fatigue-resistant low-stiffness superelastic NiTi SMA.

#### 20:15 Break

### Interdiscipline II

Chairs: TBD

#### 20:30 Contributed

### Nonadditive Strengthening Functions for Cold-worked Cubic Metals: Experiments and Constitutive Modeling

*Fulin Jiang<sup>1,2</sup>; Setsuo Takaki<sup>2</sup>; Takuro Masumura<sup>2</sup>; Ryuji Uemori<sup>2</sup>; Hui Zhang<sup>1</sup>; Toshihiro Tsuchiyama<sup>2</sup>; Fulin Jiang; <sup>1</sup>Hunnan University; <sup>2</sup>Kyushu University*

Strong metals are greatly desired for lightweight and energy-efficient industrial design. The strengthening of metals is traditionally accomplished by the additive contributions of various obstacle families (e.g., solid



solutions, particles, and grain boundaries) and dislocation self-interactions that impede dislocation motion. In the present work, unlike a traditional additive understanding, a distinctive nonadditive strengthening mixture rule for obstacles and dislocations were validated based on experimental and modeling analyses in numerous cold-worked steels and aluminum alloys. Concretely, numerous well-annealed body-centered cubic steels and face-centered cubic aluminum alloys were prepared, in which the hierarchical strength levels of solid solutions, grain boundaries, and/or particles were estimated. The above specimens were then cold rolled to various strain levels. Dislocation densities were quantified by utilizing X-ray diffraction line-profile-analysis, and the dislocation density was found to increase faster with an increasing strain level when a high strength was presented in well-annealed specimens. When plotting the yield stresses as a function of the square roots of the dislocation densities in massive distorted samples based on the Taylor hardening law, it is interesting to note that an approximate single linearity was obtained. Individual dislocation strengthening was found to respond to the total strength in the deformed specimens, which indicated that the full nonadditive strengthening mixture rule was employed between the obstacle families and the dislocation contributions. The mechanisms of the observed nonadditive strengthening were also discussed by implementing additional experiments and transmission electron microscopy observations. Then, the modified constitutive models based on both one and two internal parameters' Kocks-Mecking models were developed respectively, which excellently captured the effects of the various obstacle families on dislocation storage processes. The developed models also rationalized the observed nonadditive strengthening mixture rule.

**20:45 Contributed**  
**Structural and Compositional Evolution due to Phase Transformation in Metallic Alloys: Insights from Correlating Secondary Ion Mass Spectrometry and Transmission Electron Microscopy**

*Santhana Eswara<sup>1</sup>; Amarante J. Böttger<sup>2</sup>; Genevieve Kane<sup>3</sup>; Robert Hull<sup>3</sup>; Tom Wirtz<sup>1</sup>; <sup>1</sup>Luxembourg Institute of Science and Technology; <sup>2</sup>Delft University of Technology; <sup>3</sup>Rensselaer Polytechnic Institute*

High resolution structural and chemical analyses of multi-phase alloys are essential to elucidate the underlying processes that occur due to phase transformations. A thorough knowledge of the nanoscale structural and compositional evolution including nucleation and growth of new phases is necessary to optimize the macroscopic properties by tailoring the heat treatment process. Transmission Electron Microscopy (TEM) is often used for high-resolution structural and chemical analysis of materials. TEM is well-known for high-resolution structural imaging down to atomic scale. However, the conventional analytical tools associated with TEM such as Energy Dispersive X-ray Spectroscopy (EDX) or Electron Energy-Loss Spectroscopy (EELS) are inadequate for the analysis of (i) low-Z elements (e.g. hydrogen), (ii) dilute alloys (concentration < 0.1 at. %) or (iii) isotopes. In comparison, Secondary Ion Mass Spectrometry (SIMS) is a powerful tool for the analysis of all elements including isotopes and is highly sensitive to detect low concentrations down to the ppm range. For instance, we demonstrated the power of SIMS imaging for hydrogen mapping in a model Ni-Nb alloy [1]. However, the SIMS image resolution is fundamentally limited by the ion-solid interaction volume to ~10 nm. Therefore, by combining TEM and SIMS imaging high-resolution high-sensitivity analysis of materials can be achieved. We developed an in-situ TEM-SIMS instrument to enable such correlative microscopic analyses. The details related to the instrument and the correlative methodologies are described in a recent review paper [2]. In this presentation, we will discuss our results from ongoing research in the investigation of (i) hydrogen embrittlement in steels (mapping hydrogen trap sites in AerMet 100 and TWIP steel containing vanadium carbide nanoprecipitates) and (ii) microstructural, crystallographic and chemical evolution due to different thermomechanical treatments in dual-phase (alpha + beta) Ti-6Al-4V alloy. [1] Tarzimoghdam et al, Acta Mat., 109, 69-81 (2016) [2] Eswara et al, Appl. Phys. Rev., 6, 021312 (2019)

**21:00 Contributed****Diffusion-controlled Displacive Mechanism of the Decomposition Transformation in 2:17-type Sm-Co High Temperature Permanent Magnets**

*Tianyu Ma<sup>1</sup>; Xin Song<sup>1</sup>; Xianglong Zhou<sup>1</sup>; Tao Yuan<sup>1</sup>; <sup>1</sup> Xi'an Jiaotong University*

For more than 40 years, the 2:17-type Sm(Co, Fe, Cu, Zr)<sub>z</sub> (z is between 7 and 8) alloys with rhombohedral 2:17 (2:17R) cell interiors, hexagonal 1:5 (1:5H) cell boundaries and elongated Zr-rich platelets (Z-phase), have served as the strongest permanent magnets for high temperature applications. Prompted by the development of more miniaturized magnet-associated devices, considerable research activities have been directed towards further enhancing the energy product by raising Fe content. Despite their potential high (BH)<sub>max</sub>, the iron-rich Sm(Co, Fe, Cu, Zr)<sub>z</sub> magnets are facing a long-standing challenge, the H<sub>ci</sub> and (BH)<sub>max</sub> cannot be simultaneously enhanced due to the coercivity-remnance (Br) trade-off, which is analogous to the well-known strength-ductility trade-off for structural materials. In this talk, we shall answer two fundamental questions to circumvent such trade-off, i) why can't the iron-rich magnets form sufficient 1:5H cell boundaries to pin the motion of magnetic domain walls (the microstructural origin for their low coercivity)? And ii) how to promote their formation? In the past, the formation of cellular nanostructure that builds up the strong hard magnetism has been attributed merely to atomic diffusions, without considering the basal stacking period change from a double-layered hexagonal structure to a tri-layered rhombohedral one. Based on detailed HR-TEM investigations of an iron-rich Sm(Co<sub>0.67</sub>Fe<sub>0.23</sub>Cu<sub>0.07</sub>Zr<sub>0.03</sub>)<sub>7.6</sub> magnet, we firstly present a diffusion-controlled displacive mechanism to explain how the supersaturated hexagonal solid solution decomposes into the cellular nanostructure. The decomposition transition is found to be driven by forming long-range diffusion channels along the {011} pyramidal planes where the 1:5H cell boundaries occupy and by decreasing stacking fault energy that changes the stacking period. We further proposed a {001}<sub>a</sub><010><sub>3</sub> basal slip model to explain the formation of tri-layered 2:17R twins that have been extensively observed in the literature, and the formation of rhombohedral 2:17R' intermediate phase at the

cell edges of the iron-rich magnets, depending on whether the macroscopic strain is zero or not. The substitution of bigger Fe atoms for Co makes the diffusion kinetics slower, which help to understand the insufficient 1:5H cell boundaries and the 2:17R' intermediate phase in the iron-rich magnets. Based on the in-depth understanding of the phase transformation mechanism, our further investigations revealed that the 2:17R' phase located mainly at the cell edges weakens the domain wall energy gradient between the 2:17R cell interiors and 1:5 cell boundaries and is harmful for coercivity. Due to the metallurgical effect, the 2:17R ordering degree is lower at grain edge than that at the grain center, which also leads to inhomogeneous demagnetization process and poor squareness factor (it means that the large magnetization cannot be retained in a strong opposite magnetic field). Finally, by tailoring the decomposition transformation process, the 1:5H cell boundaries that act as the strongest pinning sites are enriched, and the fraction of harmful 2:17R' phase at the cell edges is reduced, giving rise to significant enhancements in both H<sub>ci</sub> and (BH)<sub>max</sub> (both are important considerations of permanent magnets for practical applications). For example, H<sub>ci</sub> and (BH)<sub>max</sub> of an iron-rich Sm(Co<sub>0.585</sub>Fe<sub>0.305</sub>Cu<sub>0.07</sub>Zr<sub>0.04</sub>)<sub>7.6</sub> magnet can be significantly enhanced from 9.0 kOe and 20.5 MGOe to 14.5 kOe and 28.02 MGOe, respectively. This work provides a feasible approach to overcome the coercivity-remnance trade-off for the 2:17-type Sm-Co-based permanent magnets.

**Zoom Room D****Atomistic Simulation I**

**Zoom link: TBD**

**Chairs: TBD**

**17:30 Invited**

**Defect Phase Diagrams as Novel Tool to Understand and Design Structural Materials with Superior Mechanical Properties**

*Joerg Neugebauer; Ali Zendegani; Jan Janssen; Liam Huber; Tilmann Hickel; MPI fuer Eisenforschung*

Controlling formation, size and thermodynamic stability of precipitates is a fundamental prerequisite to designing advanced precipitate hardened steels. Recent advances in experimental characterization techniques allow to accurately measure the alloy composition even in nano-sized precipitates. These experiments reveal that many of the precipitates show deviations from their ideal stoichiometry. Since such large deviations directly impact thermodynamic as well as mechanical stability, there is strong interest in understanding their origin. Conventionally, such deviations from stoichiometry are attributed to point defects, such as antisites or vacancies. High-resolution electron microscopy shows however a second mechanism: A high concentration of extended defects such as dislocations and stacking faults that can accommodate large amounts of alloying elements. To understand the formation and thermodynamics of such highly nonstoichiometric defects we introduce and employ the concept of defect phase diagrams. These diagrams show, in analogy to the well-established thermodynamic bulk phased diagrams, the thermodynamically most stable defect phase as function of state variables such as temperature, composition, stresses etc. The power and performance of this concept are demonstrated using the example of nonstoichiometric stacking faults in metallic alloys. Our ab initio computed defect phase diagrams provide an accurate tool to correctly predict the rich set of experimentally observed defect structures. Based on these insights we will discuss a conceptual framework of how to generalize these findings and to construct defect phase diagrams on a routine basis.

#### 17:45 Invited

### High-throughput Optimization of Finite Temperature Phase Stabilities: Concepts and Application

*Tilmann Hickel; Jan Janssen; Halil Sözen; Fritz Körmann; Sudarsan Surendralal; Mira Todorova; Joerg Neugebauer; Max-Planck-Institut fuer Eisenforschung*

While the present search for novel materials systems with ab initio high-throughput methods often aims at functional properties of individual structures and composition, their

finite temperature phase stabilities are mostly unknown. This is connected to the fact that density functional theory is designed to provide ground state properties. The extension to finite temperatures requires the consideration of vibrational, electronic, magnetic and configurational entropy contributions, for which complex simulation protocols are required. We have created a Python based framework called pyiron, which provides an integrated development environment for such protocols and allows one to upscale them for high-throughput simulations on large computer clusters. After explaining the underlying methodological concepts, we use the example of the hard-magnetic material system Ce-Fe-Ti to demonstrate the materials scientific consequences. Since the promising magnetic phase CeFe<sub>11</sub>Ti thermodynamically competes with various Laves phases, the partitioning of several additional elements and their impact on the relative phase stabilities have been considered. The insights obtained demonstrate how the screening of a large set of transition metals in the quaternary hard magnetic materials can be performed most efficiently and which alloying elements improve the stability of CeFe<sub>11</sub>Ti most substantially.

#### 18:15 Break

### Atomistic Simulation II

Chairs: TBD

#### 19:15 Contributed

### First-Principles Study of Phase Transformations in Zirconia: Electronic Structure, Phonon Dispersion and Symmetry Analysis

*Ying CHEN<sup>1</sup>; Lei WANG<sup>2</sup>; Tetsuo MOHR<sup>3</sup>; <sup>1</sup>Tohoku University; <sup>2</sup>University of Science and Technology Beijing; <sup>3</sup>Tohoku University*

Zirconia has three phases and the phase transformations happen from cubic (c) to tetragonal (t) then to monoclinic (m) structure with decreasing the temperature. An integrated study combined the first-principles calculations and the symmetry analysis from the space group theory brings a new

insight into the feature and mechanism of such temperature-induced phase transformations in zirconia. Based on electronic structures and phonon dispersions, the volumes and the coefficients of thermal expansion of zirconia are evaluated up to 3000K, which show the evidence of the 1st order transition for both the c-t and t-m phase transformations. Furthermore, the detailed analysis of the phonon dispersions and the c-t, t-m phase transformation path using the space group theory are conducted for each phase. The imaginary phonon frequency at Gamma point of the Brillouin zone in the higher symmetry cubic phase and the absence of this imaginary frequency with appearing the lowest frequency at Gamma point in tetragonal phase indicates this active softening phonon mode being responsible for the cubic-tetragonal phase transition with some 2nd order feature. Together with the results of coefficient of thermal expansion, some mixing feature of the 1st order and the 2nd order transformation in the c-t phase transition in zirconia is detected. Meanwhile, the analysis of the group-subgroups relationship between the tetragonal and monoclinic phase revealed that the space group of the monoclinic structure is not an isotropy subgroup of the space group of the tetragonal structure, indicating no primary phonon mode which could drive the direct t-m phase transformation and the transition might be driven by a combination of several phonon modes which matches the feature of the 1st order phase transformation.

### 19:30 Invited

#### The Phase Diagram of All Inorganic Materials

*Chris Wolverton<sup>1</sup>; <sup>1</sup>Northwestern University*

One of the holy grails of materials science, unlocking structure-property relationships, has largely been pursued via bottom-up investigations of how the arrangement of atoms and interatomic bonding in a material determine its macroscopic behavior. Here we consider a complementary approach, a top-down study of the organizational structure of networks of materials, based on the interaction between materials themselves. We demonstrate the utility of applying network theory to materials science in two applications: First, we unravel the complete “phase stability network of all inorganic materials” as a densely-connected complex network of 21,000 thermodynamically stable compounds

(nodes) interlinked by 41 million tie-lines (edges) defining their two-phase equilibria, as computed by high-throughput density functional theory. Using the connectivity of nodes in this phase stability network, we derive a rational, data-driven metric for material reactivity, the “nobility index”, and quantitatively identify the noblest materials in nature. Second, we apply network theory to the problem of synthesizability of inorganic materials, a grand challenge for accelerating their discovery using computations. We use machine-learning of our network to predict the likelihood that hypothetical, computer generated materials will be amenable to successful experimental synthesis.

### 20:00 Contributed

#### A Theoretical and Simulation Study of Precipitation in an FCC/BCC System

*Jin-Yu Zhang<sup>1</sup>; Lin Yang<sup>2</sup>; Wen-Zheng Zhang<sup>1</sup>; <sup>1</sup>Tsinghua University, Beijing; <sup>2</sup>Beijing Institute of Technology*

The properties of many structural materials are strongly influenced by size, morphology, and distribution of the precipitates formed in heat-treatment processes. An in-depth understanding of precipitate formation is essential to optimizing the fabrication and performance of these materials. However, migration mechanisms of the interfaces surrounding a precipitate remains unclear despite decades of studies. Here, atomistic simulations and theoretical analyses are conducted for the interface migrations in an FCC/BCC system. The simulation reveals the fine details of nucleation and motion of the interfacial defects around a lath precipitate. The positions of interfacial dislocations during interface migration are rationalized by the generalized O-element approach. The present results indicate that the non-conservative motion of dislocations is crucial for the nucleation and migration of growth ledges, which is the key event governing the precipitate morphology. This comprehensive study of the precipitation growth crystallography provides fundamental insight into quantitative understanding of microstructure in metallic materials.

### 20:15 Break

#### Atomistic Simulation III



Chairs: TBD

### 20:30 Contributed

#### Effects of Carbon on Mechanically-Induced Martensitic Transformation in Iron by Molecular Dynamics Simulations

*Xiaoqin Ou<sup>1</sup>; Min Song<sup>1</sup>; <sup>1</sup>Central South University*

In present study, effects of carbon (~0.2 a.t.%) on the mechanically-induced phase transformations of nano-sized face centred cubic (fcc) iron were studied by molecular dynamics simulations. The simulation systems involve both single- and poly-crystalline Fe and Fe-0.2C systems. Uniaxial tension was performed on individual simulation cell at a constant strain rate of 0.01 ps<sup>-1</sup> for a total strain of 50%. Periodic boundary conditions were applied in x, y and z directions. The simulation results show that phase transformations occurred in Fe and Fe-0.2C during tensile deformation. For the single fcc crystalline in Fe and Fe-0.2C, the parent fcc phase first transformed into stacking faults, and then the body centred cubic (bcc) phase initiated from the intersection of two stacking faults. The phase transformation led to yielding of strength in both systems during the elastic deformation stage, but the strength of the Fe-0.2C crystal yielded at a smaller strain than that of the pure Fe system. For the poly-crystalline Fe and Fe-0.2C, however, the strength yielded during the elastic-plastic deformation stage, when a large number of paralleled martensitic plates grew from grain boundaries of fcc poly-crystals. Opposite to that in single-crystalline systems, the poly-crystalline Fe-0.2C system yielded at a slightly higher strength than the pure iron system. The reason may be due to the fact that the addition of C atoms increases the stacking fault energy and thus decreases phase transformation rate in the Fe-0.2C poly-crystals.

### 20:45 Invited

#### Self-organization in Materials Subjected to Irradiation: Toward a Global Perspective

*Pascal Bellon<sup>1</sup>; Robert Averback<sup>1</sup>; Shen Dillon<sup>1</sup>;*

*<sup>1</sup>University of Illinois at Urbana-Champaign*

Irradiation can drive materials into non-equilibrium states, induce phase transformations, and nanoscale structuration through self-organization. In particular, it is now well established that ion irradiation can result in the stabilization of intragranular precipitates of finite size. These intragranular nanoprecipitates could impart radiation resistance by providing a large density of interfacial sites for point defect elimination, while at the same time improving mechanical properties. Some of the fundamental underpinnings of this compositional patterning reaction are in fact similar to the stabilization of void and bubble superlattices in irradiated solids. It is intriguing to extend these analyses to possible patterning reactions at extended defects of the microstructure, such as grain boundaries and dislocations. Recent experimental and modeling results suggest for instance that irradiation can indeed trigger compositional patterning at grain boundaries and along dislocation loops, thus providing additional means to tailor the properties of irradiated materials. While compositional patterning reactions have been reported in supersaturated alloys, i.e., in alloys containing precipitates at thermodynamic equilibrium, these reactions can also proceed in undersaturated alloys, owing to coupling between point defect fluxes and solute fluxes. From a global perspective, it is likely that all these self-organized components of the microstructure are in fact coupled and competing with another. Our understanding of such a global self-organization of the microstructure is however far less developed than that of individual and isolated self-organization reactions. We will present results illustrating recent advances in addressing this challenge, using experiments, atomistic simulations and phase-field modeling. Experiments will focus on thin films alloys based on Cu-base and Ni-base binary and ternary systems irradiated with heavy ions, characterized by advanced electron microscopy and atom probe tomography. Complementary results will be presented using atomic kinetic Monte Carlo simulations and phase field simulations, focusing in particular on the possibility of compositional patterning at grain boundaries and its competition with compositional patterning in the grain interiors.

## PTM2022 E-POSTER SESSION

### Poster 1

#### Phase Stability and Precipitation in L12-strengthened CoCrNi Medium-entropy Alloys at Intermediate Temperatures:

Jieyichen Fang<sup>1</sup>; Zengbao Jiao<sup>1</sup>; <sup>1</sup>The Hong Kong Polytechnic University

Understanding phase stability and precipitation at intermediate temperatures is crucial for tailoring microstructures and mechanical properties of L12-strengthened multicomponent alloys. The precipitate type, morphology, and distribution of (CoCrNi)<sub>100-2x</sub>(AlTi)<sub>x</sub> (x=3, 5, and 7 at. %) medium-entropy alloys (MEAs) at 600-900 °C were systematically investigated through a combination of scanning electron microscopy, energy dispersive X-ray spectroscopy, X-ray diffraction, electron backscatter diffraction, and thermodynamic calculations. Our results reveal that the Al and Ti additions promote the destabilization of supersaturated fcc into L12 and  $\sigma$  phases, and the dominating phases of the MEAs change from fcc + L12 to fcc + L12 +  $\sigma$ ; and to L12 +  $\sigma$ ; + L21 phases as the Al and Ti concentrations increase. In addition, increasing the temperature leads to a change of precipitate morphology from lamellar to granular microstructures. The effects of alloying additions and aging temperature on the phase stability, precipitation behavior, and mechanical properties of the MEAs were discussed from the thermodynamic and kinetic points of view.

### Poster 2

#### Morphogenesis of Dual-Phase Steel Microstructure During Intercritical Annealing:

Clelia Couchet<sup>1,2</sup>; Sebastien Allain<sup>1</sup>; Julien Teixeira<sup>1</sup>; Guillaume Geandier<sup>1</sup>; Frederic Bonnet<sup>2</sup>; <sup>1</sup>Institut Jean Lamour; <sup>2</sup>ArcelorMittal

Morphogenesis of a conventional DP600 steel has been simulated thanks to DICTRA/Thermo-Calc software. Austenite formation kinetics, Mn-partitioning, carbide dissolution, austenite islands growth and interaction between austenite islands through the ferritic matrix were investigated in a ternary Fe-C-Mn considering several

geometries inspired by our SEM studies. The simulations were compared to SEM, optical micrography and High Energy X Ray Diffraction experiments. These experiments have been carried out on P07 beamline in PETRA III at DESY (Hambourg) with a monochromatic beam (100 keV). High flux from synchrotron source goes through the samples and fast high-throughout 2D detector (Perkin-Elmer) collects Debye-Scherrer (DS) diffraction patterns at significant rate (10 hz). Experimental transformation kinetics were obtained by a Rietveld analysis. Main transformation kinetics features were reproduced. The simulated transformation kinetics showed high sensitivity to initial geometry and Mn diffusion. This work aims to provide better understanding for austenite morphogenesis during intercritical annealing, influencing final mechanical properties of steels.

### Poster 3

#### Effect of Transformation-induced Internal Stress on Cleavage Fracture of Lath Martensite:

Yuki Kawahito<sup>1</sup>; Daisuke Fukui<sup>1</sup>; Naoki Miyazawa<sup>1</sup>; Yuki Kawahito<sup>1</sup>; <sup>1</sup>Tokyo Institute of Technology

The effect of internal stresses generated via martensitic transformation on  $\{001\}_M$  cleavage fracture of lath martensite (M) was investigated in Fe – 0.1mass%C – 5.0mass%Mn alloy. The combination of the micropillar fabrication by focused ion beam and the precise strain measurement by digital - image correlation revealed that compressive internal stresses were anisotropically developed in Bain group of the lath martensite, where martensite variants belong to the same Bain variants. And , Charpy impact testing promoted the mode I type  $\{001\}_M$  cleavage fracture at cryogenic temperature and that cleavage crack preferred to propagate through each Bain group . Furthermore, electron - back scattered diffraction analysis proved that the crack propagation took place more frequently on  $(001)_M$  rather than  $(100)_M$  in Bain lattice correspondence . These results suggest that the internal stress originated from the Bain strain leads to the anisotropy of the cleavage fracture in lath martensite.

#### Poster 4

### Turning the Distribution of Oxide Nanoparticles in 9Cr ODS Steels from Irregular to Regular Manner via the Austenite to Ferrite Transformation:

*Xiaosheng Zhou<sup>1</sup>; Jianing Zhu<sup>1</sup>; Zhigang Yang<sup>1</sup>; Chi Zhang<sup>1</sup>; Hao Chen<sup>1</sup>; <sup>1</sup>Tsinghua University*

Oxide nanoparticles are usually irregularly distributed in 9Cr oxide dispersion strengthened (ODS) steels, while here it is interestingly found the irregular distribution can be changed into regular distribution via the austenite to ferrite transformation. In some ferrite grains, planar distribution, regular curved distribution and irregular distribution of oxide nanoparticles are all observed, which is similar to the conventional interphase carbide precipitation in high strength low alloy steels. Compositions and crystal structures of these oxide particles are examined. Effects of ferrite transformation temperature on the size and sheet spacing of oxide nanoparticles are also studied, as well as the lattice planes of oxide sheets. The mobility of ferrite/austenite interphase boundaries is suggested to be related to the dissolution of small-sized oxide nanoparticles, which has a significant effect on the formation of oxide regular distribution. Two possible mechanisms are proposed to explain the oxide regular distribution: dissolution-re-precipitation mechanism and phase-boundary dragging particle mechanism.

#### Poster 5

### Study on the Modeling for Phase Transformation of Vanadium Nitrogen Microalloyed Steel:

*Baochun Zhao; Baochun Zhao; Technology Center of Angang Steel Co., Ltd.*

Thermo-mechanical simulation tests were performed on a V-N microalloyed steel under undeformed and deformed conditions by using a Gleeble-3800 thermo-mechanical simulator to study the continuous cooling transformation behaviors and phase transformation modeling. Phase transformation temperatures were determined by thermal dilation method and metallographic method. The resultant data were analyzed by regression method based on the models from previous works to discuss the validity of the

models. The results show that there are ferrite, pearlite and bainite transformation occurring in the tested steel during the continuous cooling process. And it is also revealed that deformation can promote ferrite transformation and result in a higher ferrite start temperature and bainite start temperature. Based on the models from the previous works, the calculated phase transformation temperatures of the undeformed steel agree well with the experimental ones. But the calculated phase transformation temperatures deviate from the experimental ones obtained from the deformed steel. It is worth to note that it is irrational to use the previous models to predict the bainite start temperatures. Because bainite transformation is half diffusion phase transformation and half shear transformation, its start temperature does not change with cooling rate monotonously. While the previous models are monotone functions. Moreover, the kinetic models for phase transformation were used to construct the relationship between phase transformation volume fraction and cooling rate. And the models for the volume fraction of phase transformation were constructed. Modeling for the volume fraction of ferrite, pearlite or bainite transformation reveals that the models can predict volume fraction of microstructure in the V-N microalloyed steel with a high precision.

#### Poster 6

### Phase-field Study of Microstructure Evolution Using Co-existing External Magnetic and Elastic Fields:

*Rajdip Mukherjee<sup>1</sup>; Rupesh Chafle<sup>1</sup>; Somnath Bhowmick<sup>1</sup>; <sup>1</sup>Indian Institute of Technology Kanpur*

External fields play a vital role in tailoring microstructures for obtaining the desired properties. Phase-field modelling is an ideal tool for studying the effect of external field assisted diffusion at microscopic length scales. In this study, we use a diffuse-interface model integrated with micromagnetic and micro-elastic approaches to investigate the effects of external magnetic and elastic fields on microstructure evolution under isothermal conditions. A variety of simulations are performed to parametrically study individual, as well as combined effects of these two external fields. The initial focus of the work is to observe the effect of misfit strain, applied stress and elastic inhomogeneity on

microstructure evolution under a constant magnetic field. Depending on the elastic parameters, we perceive preferential elongation, parallel or perpendicular to the applied stress. The secondary aim is to study the domain evolution and its effect on magnetic microstructures. Magnetocrystalline anisotropy alters the orientation of magnetic domains. The domains align along the easy axes of magnetization. We observe various types of domain growth for diverse precipitate morphologies. In a three-dimensional setting, these fields cater to the change of alignment and shape of the microstructural features. The interplay between the two fields governs its effect on the temporal evolution of the system under study. The resultant effect of applied elastic and magnetic fields gives an insight into tailoring the microstructure. In his classical paper, J.W.Cahn predicted that the competition between anisotropic elastic constants and magneto crystalline anisotropy dictates the shape of precipitate i.e. plate/rod-like morphology, and the overall alignment of the microstructure is governed by the external magnetic field (J.A.P. 1963). We attempt to verify our results with Cahn's theory stating the individual contributions of elastic and magnetic fields on microstructure evolution. The results from our simulations agree qualitatively with those stated by Cahn.

### Poster 7

#### Phase Field Model on Lithium Metal Plating/Stripping Process in Lithium Metal Batteries:

Rui Zhang<sup>1</sup>; Xin Shen<sup>1</sup>; Xin-Bing Cheng<sup>1</sup>; Long-Qing Chen<sup>2</sup>; Qiang Zhang<sup>1</sup>; <sup>1</sup>Tsinghua University; <sup>2</sup>The Pennsylvania State University

Lithium metal is among the most promising anode materials in future high-energy-density energy-storage-systems due to its ultrahigh theoretical specific capacity of 3860 mAh g<sup>-1</sup> and low negative electrochemical potential (-3.040 V vs. the standard hydrogen electrode). However, Li dendrite growth, "dead Li" formation and unstable solid electrolyte interphase (SEI) have hindered its practical applications. Structured lithium metal anodes, which possess customizable conductive framework for electron transfer and designable pore structures for ion transfer, have been widely proposed to settle these issues. However, the mechanisms of stable

cycling structured anodes which can guide the design of lithium metal anodes are heavily lacking due to the grand challenges of current trial-and-error investigation based on complex materials innovation. Thus, theoretical calculation such as phase field models are employed to quantitatively describe the lithium plating and stripping process in various structured lithium metal anodes. We found that the structural areal surface area linearly determines the electroplating reaction rate in the forefront kinetic process, which is limited by electron transfer in the composite Li metal anode. Meanwhile, the structural pore-volumetric surface area exhibits an inversely proportional relationship on the electroplating reaction rate in later kinetic process, which is limited by ion transfer in electrolyte. Structured lithium metal anodes with larger areal surface area and smaller pore-volumetric surface area can be much better for high rate and high capacity battery cycling. "Dead Li" problem is another critical issue in lithium metal batteries. Electroplated lithium metal will be dissolved unevenly during discharge process, especially with considerable lithium metal dendrites. The tip of a lithium dendrite will break away from bulk lithium metal, thus forming "dead Li", which cannot conduct electrons and resulting in a loss of capacity. We have simulated the electrostripping process of lithium metal anode by phase field model. The "dead Li" formation process is quantitatively simulated on different lithium metal anodes under different discharge conditions. The overpotential evolution and simulated Coulombic efficiency are summarized, based on which we can diagnose the "dead Li" condition from practical discharging voltage curves. Beyond the design and adjustment of lithium metal anodes, further experiments and simulations are required in revealing the mechanisms in lithium metal anodes, including Li plating and stripping process, dendrite growth, SEI formation and its impact, etc. These mechanism investigations are promising for high-energy-density lithium metal batteries like Li-S and Li-O<sub>2</sub> batteries.

### Poster 8

#### Clustering Phenomena in Dilute Al-Mg Alloys:

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Solute clustering has been observed in a wide variety of commercially important Al alloys during the early stages of



both natural and artificial ageing. These clusters have been reported to act as nucleation sites for the main hardening precipitate phases. Moreover, the presence of clusters may contribute directly to the strength of the alloy. Studies to date have on solute clustering phenomena in age-hardenable 2xxx, 6xxx and 7xxx Al alloys, and there is a limited number of studies available on 5xxx Al-Mg alloys, because they are generally regarded as non-heat treatable. Here, we investigate the nature of the dispersion of the Mg atoms in dilute binary Al-Mg alloys during natural and artificial ageing. Two model alloys were studied, a very dilute Al-0.01Mg (at.%) alloy and a dilute Al-0.8Mg (at.%) alloy containing ~10x more solute. After solution treatment at 450°C for 2 hours followed by water quenching, both alloys were either naturally aged or artificially aged at 175 °C for 5 min and investigated using atom probe microscopy. As expected from the phase diagram, no second phase precipitates were detected in any of the conditions studied. The as-quenched hardness of the Al-0.8Mg alloy was ~85% higher than that of pure Al, and this comparison was further increased to 115% after artificial ageing. Nonetheless, the hardness of the Al-0.01Mg alloy did not change significantly after ageing. We employed advanced cluster-searching algorithms to reveal the statistical details of the Mg solute arrangement in the Al matrix of both alloys in the various conditions. We quantify where the Mg-solute dispersion is effectively random, and where it varies from random and how the solute cluster statistics change with ageing condition and hardness values.

## Poster 9

### Study of Carbon Content Evolution in Austenite during Austenitization by in situ Synchrotron X-ray Diffraction of a Hypoeutectoid Steel:

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The weight of crankshafts for automotive industry can be reduced by surface hardening achieved by surface induction heat treatment [1],[2]. The thermal history and the phase transformations lead to compressive residual stresses at the surface combined with better mechanical properties, which

are optimal for the in-use properties of the crankshafts [3]. The initial microstructure of the steel (before the heat treatment) may affect the austenitization kinetics and microstructure evolutions due to differences in nucleation sites nature and distribution, characteristic sizes determining the diffusion distances and interstitial and substitutional elements distributions. Controlling and understanding these evolutions is essential to optimize these treatments. Even for a fully austenitic final layer, the chemical composition may present local heterogeneities due to initial microstructural features leading thus to local differences in final microstructure after the cooling with different local mechanical properties. A previous study [4] on a low-alloyed steel with composition Fe-0.36C-1.25Mn-0.7Cr-0.12V-0.07Mo (wt.%) showed the importance of the initial microstructure (ferrite-pearlite, tempered martensite and bainite) and of the heating rate on the austenite formation kinetics. The utilization of High Energy synchrotron X-Ray Diffraction (HE-XRD) [5] allowed to characterize the phase fraction evolution of all phases and highlighted two steps in the austenite formation: i) the simultaneous transformation of ferrite and dissolution of cementite into austenite, and ii) the transformation of the remaining ferrite into austenite. For a given heating rate, the kinetics of each step was shown to be dependent on the initial microstructure. In addition to the nature and the amount of phases formed, the Rietveld refinement [6] of diffraction patterns also gives information's about the lattice parameters and widths of diffractions peaks for different phases at any time during heating and the austenite formation. To get insight into the phase transformation mechanisms, the present paper focuses on the evolution of lattice parameters of austenite, ferrite and cementite to be able to estimate the chemical composition evolution in these phases for the three different initial microstructures on heating at 0.25, 10 and 100 °C/s. It is shown that the lattice parameters of ferrite, cementite and austenite do not vary linearly with the temperature, especially, in the temperature range where the austenitization takes place. Since the austenite has a low yield stress in the temperature range where the transformation occurs, low internal stresses can be assumed and the changes in its lattice parameters should be mainly associated with chemical composition variations. Moreover,

the carbon contribution to the austenite lattice parameter is shown to be 10 times higher than that of substitutional elements. Therefore, it is suggested that the deviation from the linearity is mainly associated with the carbon content variation inside the austenite. Using Dyson and Holmes equation [7], the carbon content in austenite is estimated for any moment of the austenite formation for each initial microstructure and all heating rates. For example, for the ferrite-pearlite microstructure heated at  $0.25^{\circ}\text{C}\cdot\text{s}^{-1}$ , the carbon content in austenite after complete cementite dissolution corresponds to that of pearlite. For all initial microstructures, a rapid decrease in carbon content in the austenite is observed during the first stage of the austenitisation (simultaneous dissolution of ferrite and cementite) followed by a slow further decrease during the transformation of the remaining ferrite resulting in a decrease of the mean lattice parameter of austenite. We show also that the initial mean carbon content in austenite at the beginning of the austenite formation is dependent on the heating rate: it decreases as heating rate increases. The values of initial carbon content in the first austenite formed are in good agreement with thermodynamic calculations. References: [1] Desalos Y, Le Strat F. Techniques de l'Ingénieur (in French), M1205 (1996) 1-25 [2] Barglik J, A. COMPEL - The international journal for computation and mathematics in electrical and electronic engineering, Vol. 36 (2017) Issue: 2, 555-564 [3] Kabasakaloglu U, Saruhan H. Materials Testing Vol. 61 (2019) Issue: 3 277-281 [4] Esin VA, Denand B, Le Bihan Q, Dehmas M, Teixeira J, Geandier G, Denis S, Sourmail T, Aeby-Gautier E. Acta Materialia 80 (2014) 118-131 [5] G. Geandier, E. Aeby-Gautier, A. Settefrati, M. Dehmas, B. Appolaire : C. R. Physique, 13 (2012) 257-267 [6] H.M. Rietveld : J. Appl. Cryst., 2 (1969) 65-71 [7] D.J. Dyson and B. Holmes: J. Iron Steel Inst., 208 (1970), 469

### Poster 10

#### Effect of Short-Range Diffusion Phase Transformation in Co-Ni-Cr-Mo alloy:

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MP35N alloy has composition Co-35Ni-20Cr-10Mo and it can be formed into multiple forms such as plate, sheet, rod, and wire. One application of MP35N in medical devices is

to draw a fine wire as a conductor. A lead is a conductor system which transfer electrical signal from a medical device, such as a Pacemaker, to the targeted area such as left ventricle in heart. A lead is consisted of electrodes, insulator and conductor wire. The MP35N wire has been used to make leads conductor in medical devices for more than 30 years because of its high fatigue properties, good corrosion resistance and conductivity. However, the phase transformation has little been studied. The reported phase transformation on MP35N was based on thick plate samples which usually has a long dwelling time at elevated temperatures. The fine wire drawing processes of MP35N has a much shorter time and temperature than plate form of MP35N. The additional process on wire such as insulating coatings can have a strong effect on wire properties. This work is to study the phase transformation on the wire form of MP35N. It was observed that tensile strength increases with cold work and aging temperature. Tensile modulus increases with the aging temperature. The resistivity increases with aging temperature. The aging effect occurred under a short of time. Tensile strength increases in a few seconds at elevated temperature aging process. TEM study indicates that no precipitation was observed after aging process. A proposed mechanism of the phase transformation in MP35N is alloy elements segregation on defects by short range diffusion.

### Poster 11

#### The role of interfacial coherency in the kinetics of austenite to ferrite transformation in Fe-C-M alloys: a phase field study:

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A phase field model with a treatment of non-steady-state segregation of substitutional alloying element is developed to study the role of interfacial coherency on  $\gamma$  to  $\alpha$  transformation kinetics in ternary Fe-C-M alloys (where M is the substitutional alloying element). The developed model can physically describe the element partitioning and segregation simultaneously during the migration of  $\alpha/\gamma$  interface with various interfacial coherencies. The comparison of experimental data and simulation results demonstrates that the kinetics of  $\gamma$  to  $\alpha$  transformation in

ternary Fe-C-M alloys should be determined by the migration of both non-coherent and partly-coherent interfaces, and the conventional belief that the  $\gamma$  to  $\alpha$  transformation kinetics is dominantly decided by the migration of non-coherent interface is found to be an extreme case of the developed phase field model. Furthermore, the model predicts a competitive relationship between non-coherent and partly-coherent interfaces during  $\gamma$  to  $\alpha$  transformation in Fe-C-M alloys and the competition is significantly affected by the type as well as the content of substitutional alloying elements.

### Poster 12

#### Flash Annealing of Interphase Precipitation Steels: Microstructure and Mechanical Properties:

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Fasting annealing (FA) is a cost-effective heat treatment to benefit the mechanical properties of various multi-phase advanced high strength steels, while its application to the fully ferritic steels receives quite less attentions. Here we explore the potential roles of FA in the microstructure and mechanical behavior of a cold-rolled Ti-Mo containing ferritic steel strengthened by interphase-precipitated alloy carbides. It was interestingly found that the combined use of FA and strong pinning effects by pre-embedded nanosized carbides can result in a heterogeneous ferritic matrix consisting of soft recrystallized/transformed and hard non-recrystallized/transformed ultrafine domains. which brings an intense bask-stress hardening. As compared with the as-received steel, the FA-treated steel exhibits a much higher ultimate tensile strength without great loss in ductility. FA opens a new route to tailor the microstructure and optimize the mechanical performance of ferritic nanoprecipitate-strengthened steels.

### Poster 13

#### In-situ Measurement and Modeling of Deformation-induced Martensitic Transformation in a Metastable Austenitic Stainless Steel under Cyclic Loadings:

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In the present paper, deformation-induced martensitic transformation under cyclic loading in metastable austenitic steel AISI 348 was in-situ monitored through the magnetic permeability method with a Feritscope. Stepwise cyclic loading tests under room temperature revealed nonlinear and non-monotonic variations of the magnetic permeability within single loading cycles. The magnetic response was confirmed to be influenced by plastic deformation and internal stresses. A phenomenological model was proposed to correlate the Feritscope output with effective stress. The band-like structure of martensite was observed along the principal stress axis and forming a material with composite nature. A stress partitioning model based on the dual-phase concept was established and the macroscopic stress is distributed in constituent phases. Mechanical behaviors of both phases were modeled the cyclic plasticity and the obtained stress-strain curves match well with the experimental results. On knowing the evolutions of internal stresses in the martensitic phase, the variations of magnetic properties under both loaded and unloaded states were well modeled.

### Poster 14

#### Revealing the Effects of Mo and W on Carbide Precipitation in Austenite of Microalloyed Low Carbon Steels:

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Mo and W are two important alloying elements in steels, and they play the similar role in influencing phase transformation and carbide precipitation. On the one hand, Mo and W can influence the austenite decomposition, thus medium or low temperature transformed products e.g. bainite or martensite can be obtained. On the other hand, secondary hardening occur by forming carbide of Mo or W (e.g. M<sub>2</sub>C) during tempering below A<sub>1</sub>. In recent years, Mo and W are added into Ti or Nb microalloyed steels, and refined MC-type complex carbide particles (M=Mo, W, Ti, Nb) precipitate and correspondingly the precipitation hardening is enhanced obviously. Although Mo and W are thermodynamically unfavorable in forming MC-type carbide, and M<sub>2</sub>C-type carbide has very large solubility in austenite, Mo and W

were found to incorporate into TiC (or NbC) carbide in austenite of Ti or Nb microalloyed steel in our recent works. First principle calculations show that the incorporation of Mo (or W) in TiC (or NbC) can remarkably reduce the interfacial chemical energy of TiC/ $\gamma$ , thus the complex MC carbide can be formed. Interestingly, Mo and W are found to segregate at outer layer of MC particle, forming a “core-shell” structure, which verify the results of first-principle calculations.

## Poster 15

### Response of Molybdenum Alloys to Gaseous Nitriding at Elevated Temperatures:

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Molybdenum alloys (Mo-Ti and Mo-V with the Ti/V atomic range between 5-25 at.%) were applied to investigate their response to internal gaseous nitriding in terms of layer formation and hardening at elevated temperatures between 700 °C- 1100 °C using various times. The gaseous nitriding medium containing Forming gas (95 % N<sub>2</sub> and 5 % H<sub>2</sub>) with the gas flow rate of 60 l/h were applied. A diffusion zone of around 15  $\mu$ m was formed after nitriding treatment at 1100 °C for 10 h. X-ray diffraction patterns recorded from surface of nitrided specimens depict the formation of VN nitride on the surface of Mo-V and TiN nitride and minor amount of TiO<sub>2</sub> oxide on the surface of Mo-Ti alloys. Nitrided layer shows an increased hardness of around 1400 HV0.01 near surface areas. On a prolonged treatment time and for the alloys containing higher amounts of alloying elements a coarsening of TiN/VN precipitates occurs, in particular by a discontinuous coarsening mechanism, involving growth of Mo and TiN/VN lamellae from the nucleation sites such as surfaces and grain boundaries.