# Fundamentals of SIMS – From nanocraters to gas phase ions

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

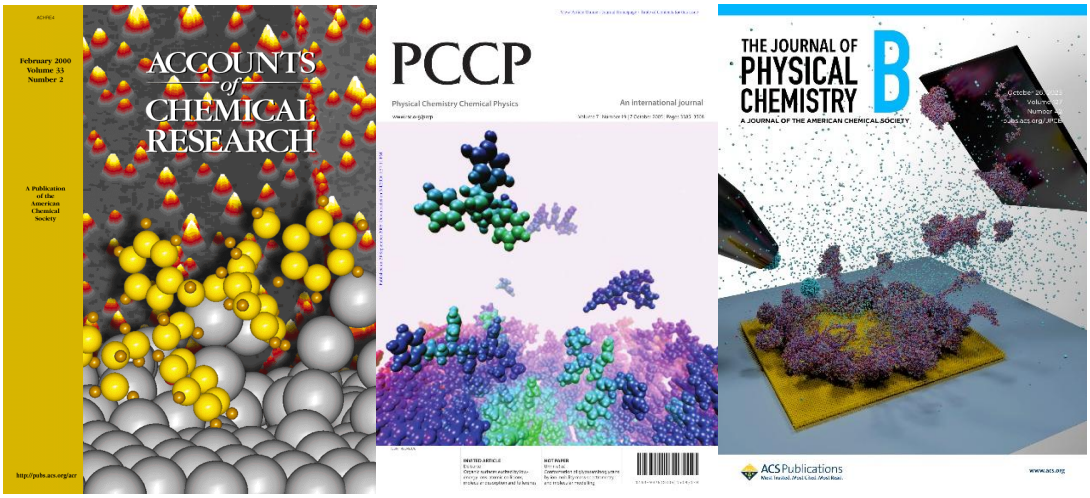


*Figure 1. Views of the molecular dynamics from published articles. (A) Emission of polystyrene oligomers adsorbed on Ag induced by 500 eV Ar projectiles (2000). (B) Desorption from a bulk PS molecular solid under 5 keV Ar impact (2005). (C) Crater formation and molecular emission from an enzyme film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

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