Exploring SIMS-Related Phenomena through Recent Computer Simulations

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

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

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

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