

Large gas cluster impacts with organic surfaces: From nanoscopic physics to 3D molecular imaging

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Synopsis This contribution focuses on the interaction of keV gas clusters with organic surfaces. The physics of crater formation, molecular sputtering and fragmentation is elucidated using a combination of computer simulations and experiments. The application for 3D molecular analysis of surfaces and thin films is demonstrated.

Over the past decades SIMS has moved from probing and imaging surfaces with keV atomic ions to small clusters such as SF_5^+ , C_{60}^+ or Bi_n^+ and, most recently, to nanoparticles like Ar_n^+ or $(\text{H}_2\text{O})_n^+$ containing thousands of atoms. This shift in projectile size involves a shift of underlying physical processes, from linear collision cascades to collective atomic motions and macroscopic-like impact phenomena.

In this contribution, we first use the results of molecular dynamics (MD) simulations [1] and experiments to elucidate the qualitative and quantitative changes associated to this increase in projectile size, which translates in ever smaller energies per projectile mass unit – eV/amu, and gives rise to a regime in which sample molecules are emitted without fragmentation (Figure 1). The positive consequences are illustrated, e.g. the possibility of soft sputtering and molecular depth-profiling, giving unprecedented information on the chemistry changes at

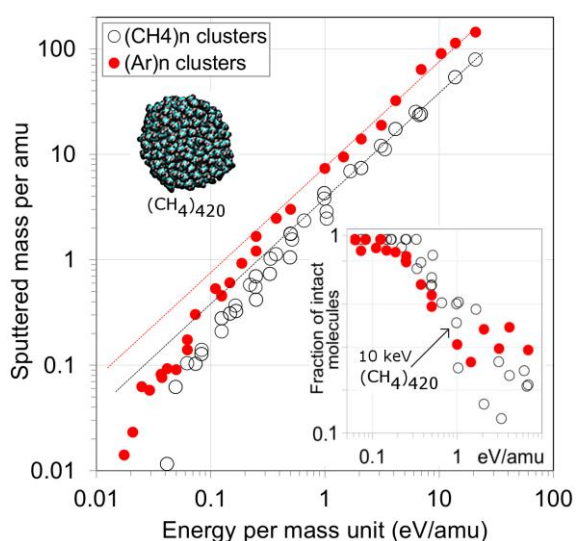


Figure 1. Calculated dependence of the scaled sputtered masses of polyethylene oligomers on the scaled kinetic energy for $(\text{CH}_4)_n$ and Ar_n clusters. *Inset:* Energy-dependence of the fraction of the mass sputtered as intact molecules.

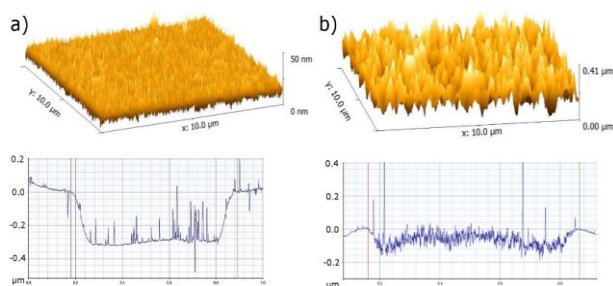


Figure 2. AFM topography and stylus profilometer profile of 10 keV Ar_{3000} sputtered surface areas in (a) pure polycarbonate and (b) polycarbonate loaded with 10 wt.% nanoparticles (same primary ion dose).

the nanometer-scale in fully organic thin films (OPV and OLED multilayers, plasma-treated polymers [2]), but also the negative effects, e.g. a very large sputter yield difference between organic and inorganic materials generating undesired topography in the 3D analysis of hybrid multilayered or composite samples (Figure 2).

For organic layers bombarded by large gas clusters, variations of sputter yield depending on the molecular size and substrate nature are also observed in the experiments and explained by the models. Interestingly, the backscattering of gas cluster fragments also provides information on the local mechanical properties of the bombarded surface [3], which will be shown here for the first time for organic solids. This potentially adds a new dimension to SIMS imaging with large clusters.

References

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