Simulation of (bi-)metallic cluster growth on polymer surfaces during sputter deposition

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Plasma-based physical vapor deposition methods are frequently used to fabricate metal-polymer nanocomposites. Aiming at the production of nanoparticles with tailored optoelectronic properties, one has to understand how crucial cluster properties such as composition, size and shape evolve in the self-organized growth process. While computer simulations are helpful to gain insight into the growth behavior, the required time scales still impose big challenges on all currently available methods. In this work, we present an accelerated Langevin dynamics method that we apply to simulate the growth of Au clusters and bi-metallic Ag-Cu clusters on polymer surfaces [1]. The simulation scheme comprises the deposition of metal atoms, diffusion of the particles on the surface, desorption of atoms as well the creation of surface defects caused by the impingement of highly energetic ions that are emitted from the plasma. We show that our results for Au particles are in good agreement with recent GISAXS experiments [2] and we demonstrate how the UV-Vis absorption spectra can be calculated for simulated Ag-Cu particles.

References