Growth of metal nanoparticles in a polymer thin film: a molecular dynamics approach based on Langevin's equation

Tim Willame , Clémence Mimoso , Sabrina Devouge , Corentin Guyot , and Michel Voué*[1]

[1]Université de Mons (LPMO) – 20, place du Parc, B7000 Mons, Belgique

Résumé

Since the pioneering work of Porel and colleagues, polyvinyl alcohol (PVA) thin films doped with in situ grown silver clusters have become a fascinating model for investigating the optical properties of plasmonic nanocomposite materials. Our recent studies have demonstrated that maintaining a constant metal-to-polymer ratio, but altering the polymer dilution or adjusting the spin coating conditions to produce films of decreasing thickness, consistently results in a red-shift of the plasmon resonance. This phenomenon appears to be independent of the polymer's molecular weight and may be attributed to substrate effects or the influence of film thickness on the growth mechanism. In this study, we present a molecular dynamics approach based on Langevin's equation, addressing the problem of the aggregation of diffusing tracers. This approach simulates the diffusion of neutral metal atoms within the polymer matrix. The simulations, conducted using the LAMMPS software, examine the morphological characteristics of the clusters as a function of film thickness, tracer interactions, and the friction between tracers and the matrix. They show that in the thinnest films, the clusters are asymmetric, corresponding more to a 2D growth mecanins than to a 3D one which occurs in the thicker ones.

Mots-Clés: molecular dynamics, Langevin's equation, spectroscopic ellipsometry, plasmon resonance, plasmonic nanocomposite materials

*Intervenant