Molecular Dynamics Simulations of P3HT Multilayer under Low-Energy Monoatomic Projectile Bombardment

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Poly(3-hexylthiophene) P3HT is a widely studied conjugated polymer with interesting properties that makes it a versatile organic material for various applications [1]. However, several technological challenges still exist for using it in a large-scale. The improvement of devices, including this type of materials relies on an appropriate analytical technique capable of making the link between their structural and chemical features and their operational performance. As devices are generally multilayer structures, ToF-SIMS may have an important role to play for the improvement of these materials [2]. However, the choice of projectile used for sputtering, their kinetic energy, angle of incidence, etc. are essential factors affecting the sputtering. Therefore, molecular dynamics (MD) simulations could help overcoming those issues through elucidating the mechanisms of ejection [3].

In this contribution, we investigate the sputtering behavior of P3HT deposited on a silicon substrate under low-energy monoatomic (He, Ar and Xe) projectile bombardment using MD simulations. The effect of the organic overlayer thickness on the sputtering efficiency and structural and chemical damage induced in P3HT under the conditions usually used during SIMS analysis of these materials with low-energy atomic projectiles will be discussed. The 500 eV He, Ar, and Xe projectiles at a 45° impact angle are employed to gain insights into sputtering and material modification mechanisms. The effect of the primary kinetic energy and the impact angle of the Ar projectile on the sputtering efficiency will also be reviewed.

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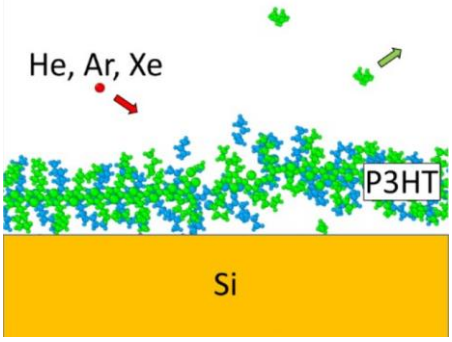

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