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Molecular dynamics computer simulations of 5 keV C₆₀ bombardment of benzene crystal

Bartłomiej Czerwiński¹⁾, Łukasz Rzeźnik¹⁾, Robert Paruch¹⁾, Edward J. Smiley²⁾, Barbara J. Garrison²⁾, and Zbigniew Postawa¹⁾

¹⁾ Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Kraków, Poland ²⁾ Department of Chemistry, The Pennsylvania State University, University Park, PA 16802, USA

Coarse-grained molecular dynamics computer simulations have been used to investigate the damage of thick benzene crystal induced by 5 keV C_{60} projectile bombardment. The sputtering yield, mass distributions and the depth distributions of ejected organic molecules are analyzed. The temporal evolution of the system reveals that impinging C_{60} cluster leads to creation of almost hemispherical crater. Most of the molecules damaged by the projectile impact is ejected into the vacuum during cluster irradiation. Similar behavior does not occur during atomic bombardment where a large portion of fragmented benzene molecules remains inside the crystal after projectile impact. This "cleaning up" effect explains why secondary ion mass spectrometry (SIMS) analysis of organic samples with cluster projectiles can produce significantly less accumulated damage compared to analysis performed with atomic ion beams.