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Molecular Dynamics Simulations to Explore the Effects of Si-C Chemistry in 20-keV C60 Bombardment of Si CLARISSA BRINER[1], KRISTIN KRANTZMAN[2], College of Charleston — C_{60} ion beams have been successful for high resolution sputter depth profiling of metallic multilayer structures. However, in experiments of C_{60}^+ bombardment of Si, unusual effects are observed, which are thought to be due to the strong covalent bonds that can be formed between C atoms from the projectile and Si atoms from the substrate. Similar effects have been observed in experiments on organic materials with C_{60}^+ projectile. We have adopted a recently developed scheme to model multi-impact bombardment of C_{60} on a single Si surface. Recent experiments have shown that C atoms are primarily ejected in the form Si_3C^+, a result which has led the authors to conclude that C atoms from the projectile are incorporated into the substrate by bonding to three neighboring Si atoms. We present the results of molecular dynamics (MD) simulations to model cumulative effects of successive C_{60} bombardment. Analysis has been done on composition of sputtered clusters, cluster ejection mechanisms, and surface composition by layer depth.

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