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Investigation of Interactions of Atomic Hydrogen with Amorphous Carbon Films BHAVIN N. JARIWALA, CRISTIAN V. CIOBANU, SUMIT AGARWAL, Colorado School of Mines — Hydrogenated amorphous carbon (a-C:H) films are generally deposited using plasma enhanced chemical vapor deposition from hydrocarbon feed gases. The structure and properties of these films are defined by the sp^2-to-sp^3 hybridization ratio and the H content. Interaction of H generated in the plasma results in local and overall transformations to a diamond-like structure due to various reactions. We have employed classical molecular-dynamics (MD) simulations based on the modified extended Brenner potential and experiments to study atomic H interactions with a-C:H thin films. Using MD, we first developed a procedure for creating realistic a-C:H thin films and formulated a scheme to characterize the sp^2-to-sp^3 hybridization ratio. These films were then impinged with H atoms at random locations and the specific chemical reactions of the H atoms with the a-C:H surface were identified through a detailed analysis of the MD trajectories. The reaction mechanisms for the hydrogenation reaction, H-atom abstraction and chemical erosion through desorption of stable hydrocarbon species have been identified and shown to be consistent with experimental measurements. Support from NSF award number DMR-0820518 is gratefully acknowledged.

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