

Abstract Submitted
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Molecular Dynamics Simulation of Chemical Sputtering¹ S.J. STUART, Department of Chemistry, Clemson University, SC, P.S. KRSTIC, C.O. REINHOLD, Physics Division, ORNL — We study chemical sputtering by D and D₂(*v*) at deuterated amorphous carbon surface. The dynamics of the surface characteristics is a function of the initial surface and the cumulative effect of the projectiles. We study evolution of the spectrum of the sputtered particles, hydrocarbons, in search for the steady “state” sputtering yield. The comparison of the steady yields of atoms vs. molecular projectiles in various vibrationally excited states enables interpretation of the ORNL experimental results.

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