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Chemical Sputtering of Carbon Revisited: Temperature and Isotope Effects¹ JONNY DADRAS, University of Tennessee, CARLOS REINHOLD, PREDRAG KRSTIC, Oak Ridge National Laboratory — We study chemical sputtering of carbon irradiated by 1-30 eV/D atoms, in a range of temperatures, 300 – 1200 K by molecular dynamics, using modified potentials of Brenner-Terzoff type. At each temperature and impact energy a quasi-stationary state of the carbon erosion is reached by cumulative bombardment. Dependence of the mass and energy spectra of hydrocarbons, as well as the moiety density (sp, sp², sp³), on surface temperature are studied. We also study the chemical erosion of hydrogen-supersaturated carbon kept at 300K due to bombardment by hydrogen isotopes H, D, and T at energies of 1–30 eV. Chemical sputtering yields are found to increase with projectile mass but not as dramatically as that predicted by simpler models based on sequential binary collisions. Only a weak dependence on the mass was found in the number of hydrocarbon moieties of supersaturated surfaces created by cumulative bombardment and, thus, the root of the mass dependence was found to be directly related to the probability for breaking the C–C bonds that attach such moieties. Our results are compared with available experimental data on acetylene, methane, and total carbon sputtering yields.

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