Computer Simulation of Chemical Sputtering of Carbon Surfaces by D2 and D

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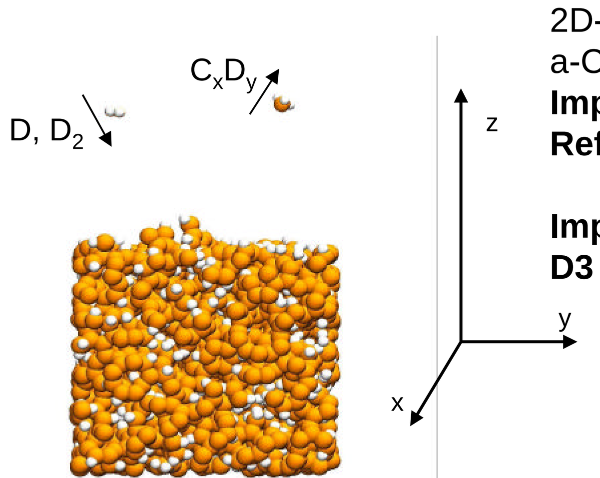
Chemical sputtering of carbon by D and D_2 impact is studied at impact energies ranging from 7.5 to 30eV/D using molecular dynamics simulations that mimic, as closely as possible, particle beam experiments. The substrate structure is heavily modified by cumulative impacts, and the sputtering yields change with bombardment time, eventually reaching a quasi steady state. The yields of the hydrocarbons in this quasi-steady-state regime are in good agreement with experiment, and are significantly larger and of different structure than those from the unmodified surfaces. Analysis of the steady-state yields from projectiles in various vibrationally excited states, enables interpretation of recent experiments. six surfaces are prepared at each energy and each type of projectile in the transient steady state regime.

System & potentials

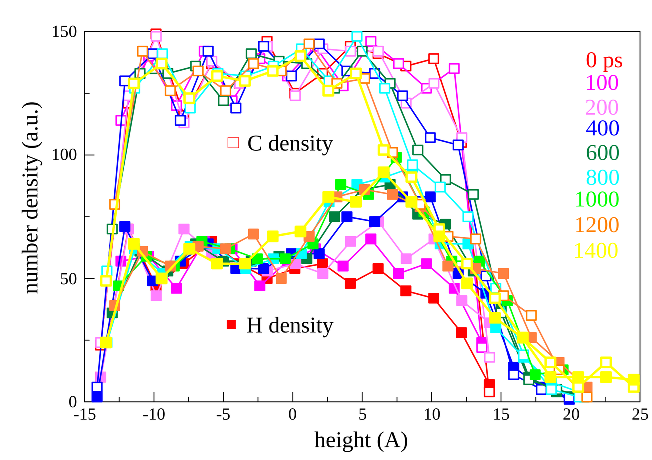


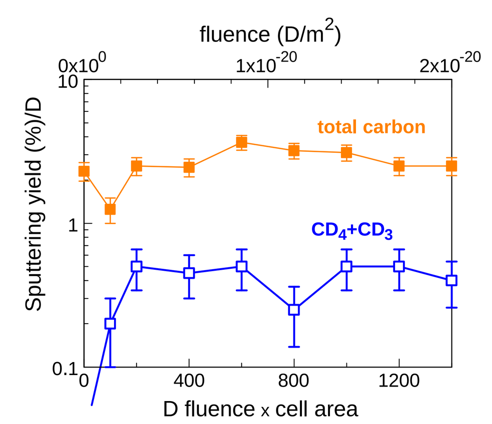
2D-periodic
a-C:D surface
Improved REBO potential, Ref. 1

Impact of D, D2 (exc.) and D3 (diss.)

Impact orthogonal to the surface
Random uniform emitting plane, molecular orientation random, Rotational T~1000K

Surface Preparation

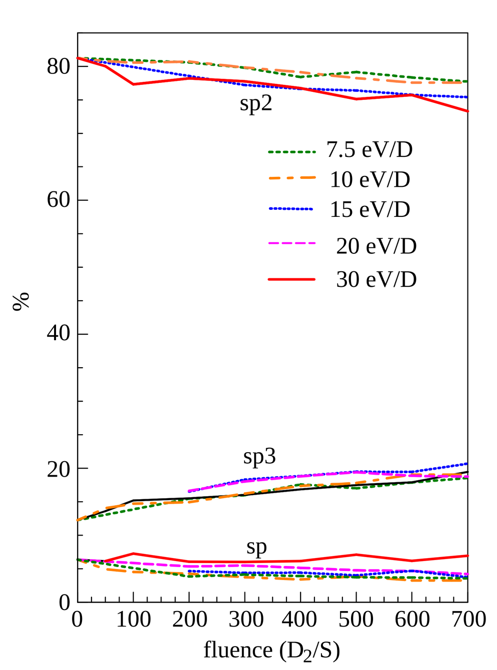


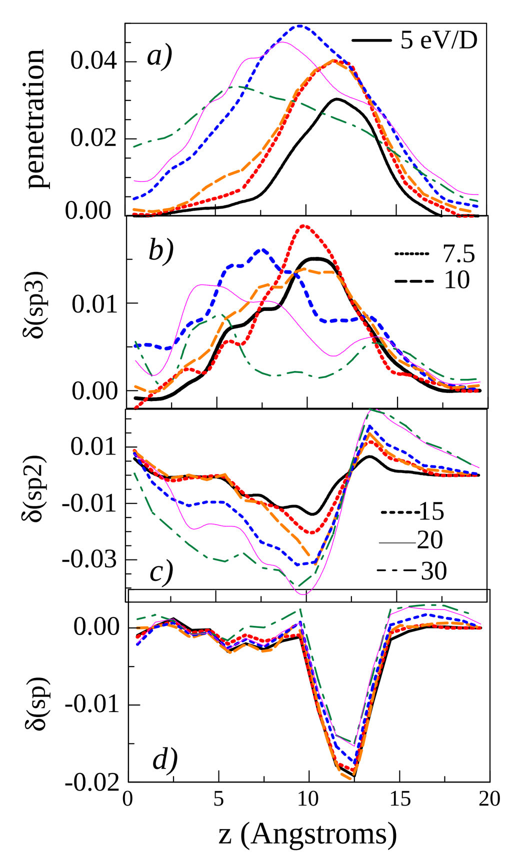


Steady!

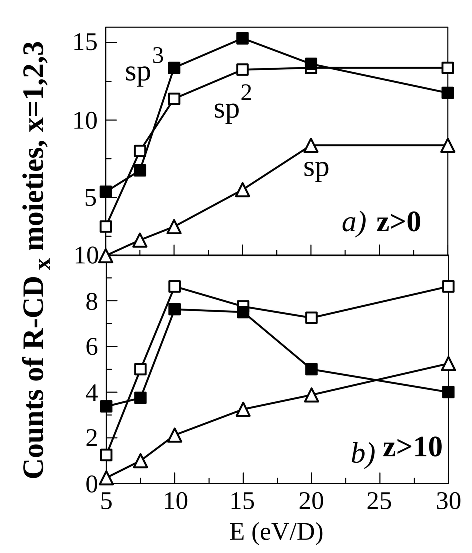
An initial 2D-periodic a-C:D surface with N_H/N_C = 0.40 was bombarded with D or D_2 projectiles at normal incidence, and at a flux of ~10^{28} m^{-2} s^{-1} (2 ps between impacts) using forced thermal relaxation between impacts. Total fluences of up to ~2 × 10^{20} m^{-2} (1000 impacts) were achieved.

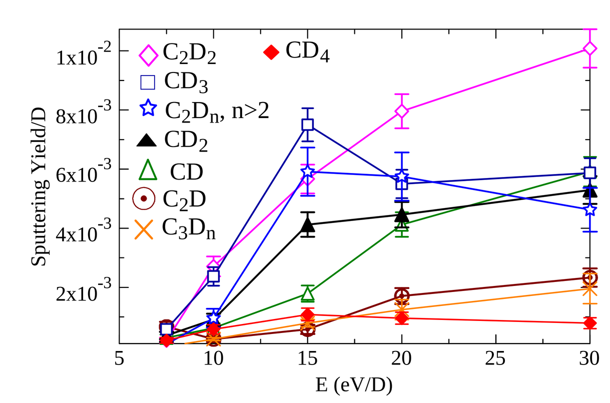
Surface Structure





The damaged surface is very different from bulk a-C:D, and becomes supersaturated with deuterium with increasing fluence (eventually reaching a transient saturation regime). Supersaturation with deuterium is confined to the outermost 15 Å of the surface. The H/C ratio reaches 1.0 in this surface layer. More saturated complexes are formed which give rise to new sputtered species.

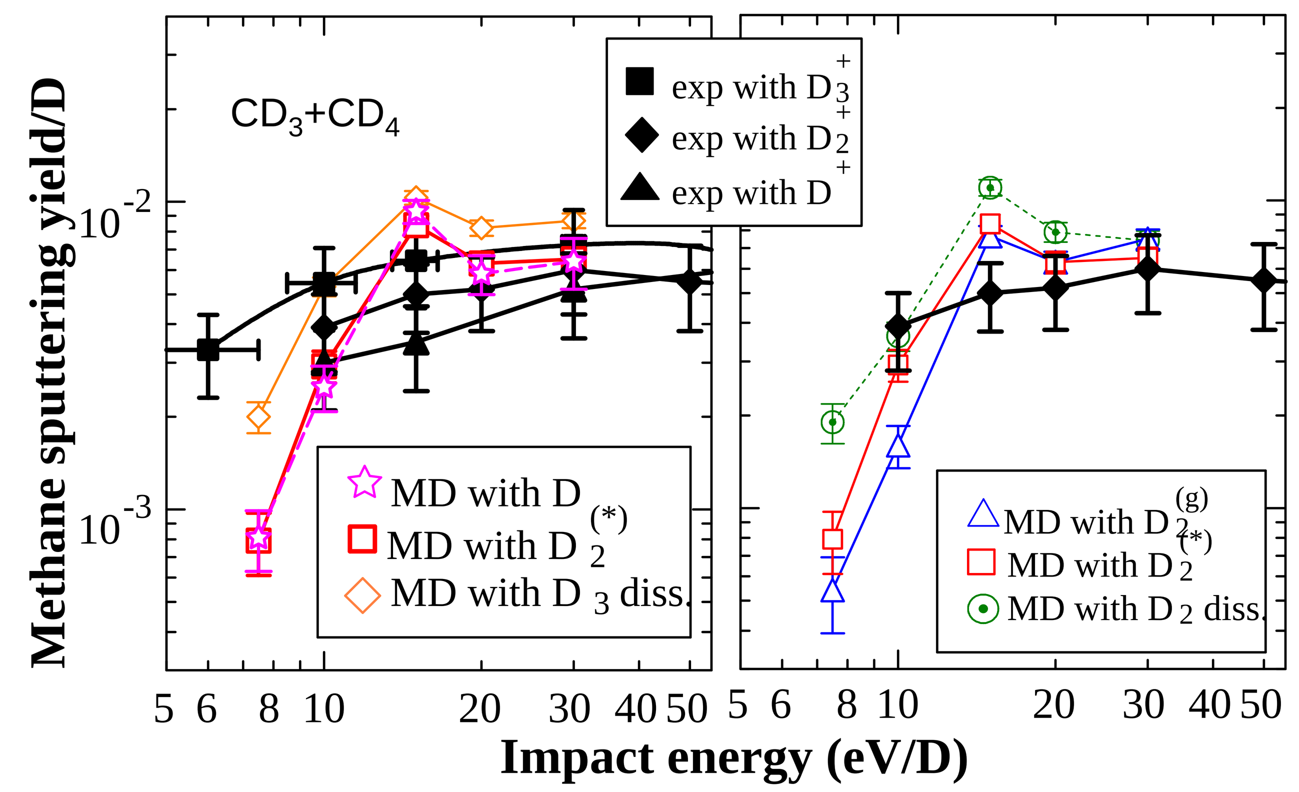




The ejecta from the damaged surface are very different from those of the initial surface, and include more molecular and saturated species. The yield dependence on impact energy follows sp3, sp2, sp contents.

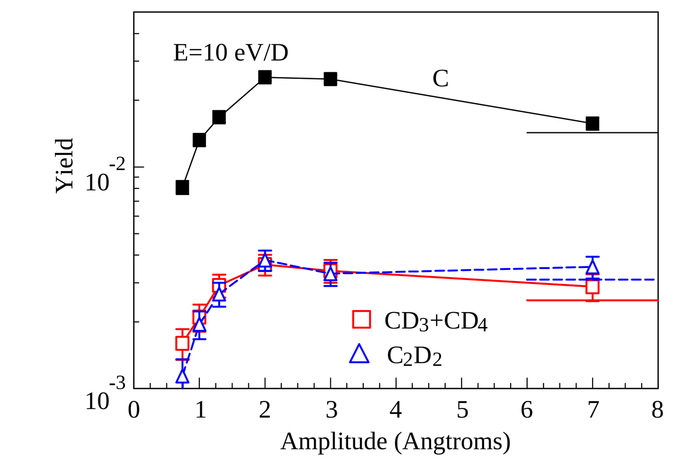
Effects of atomic and molecular projectiles (in the ground or a vibrationally excited state) are visible and may explain experimental findings [2]. Our simulations indicate that it is both feasible and necessary to perform sputtering simulations on surfaces that have been dynamically created by impacts, rather than equilibrium surfaces, if meaningful comparison with experiment is desired.

Comparison with Experiment

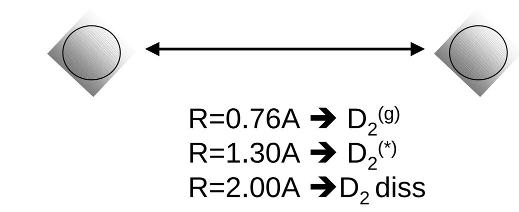


Beam experiments at ATJ graphite, of F. W. Meyer (Ref. 2)

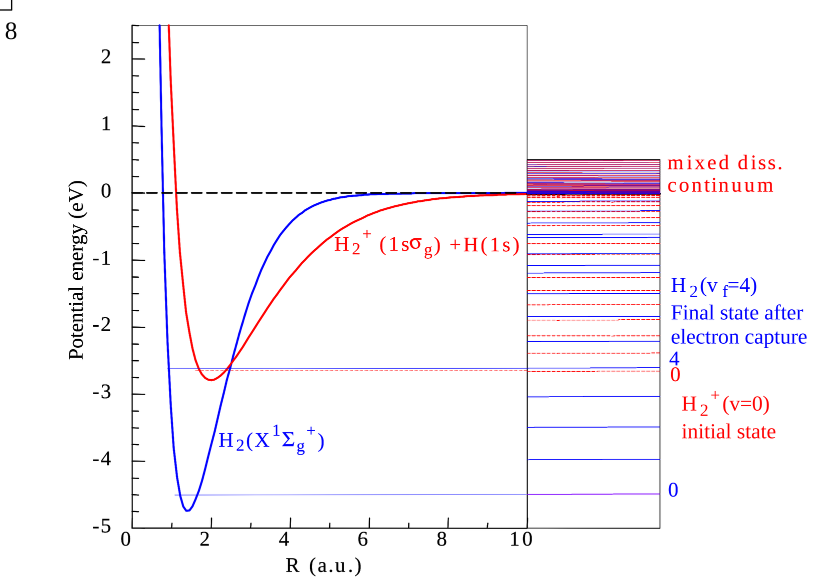
Effect of Projectile Vibrations



Sputter yields of all species increase with vibrational excitation of the impinging molecular projectile !!!

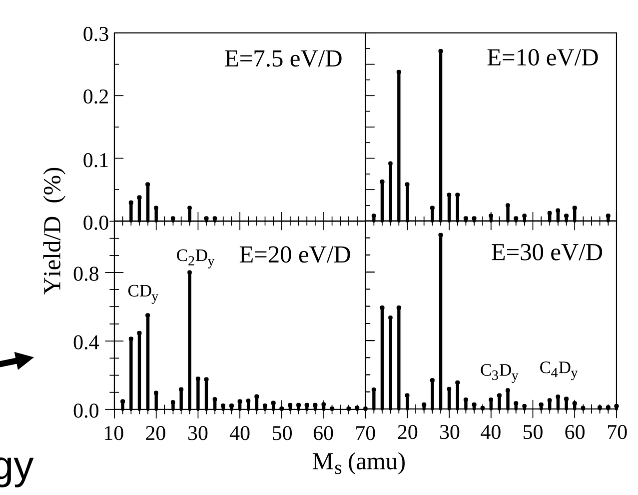


Ion Neutralization

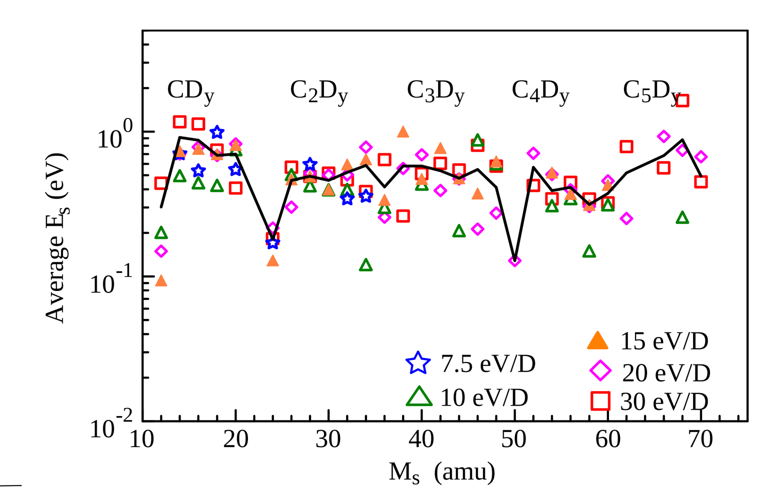


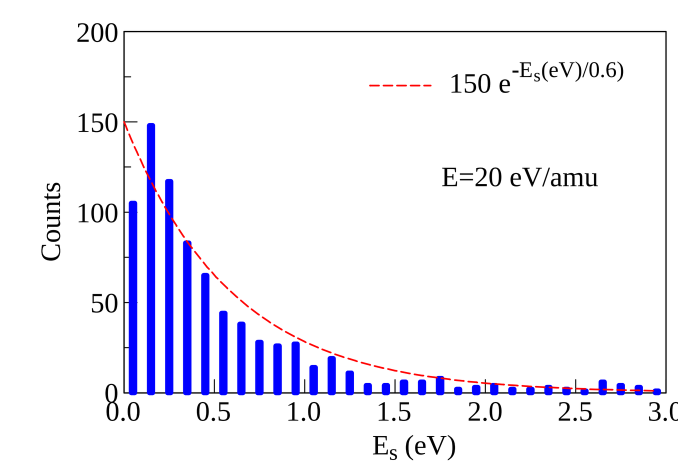
Sputtered Spectra

Heavier with energy

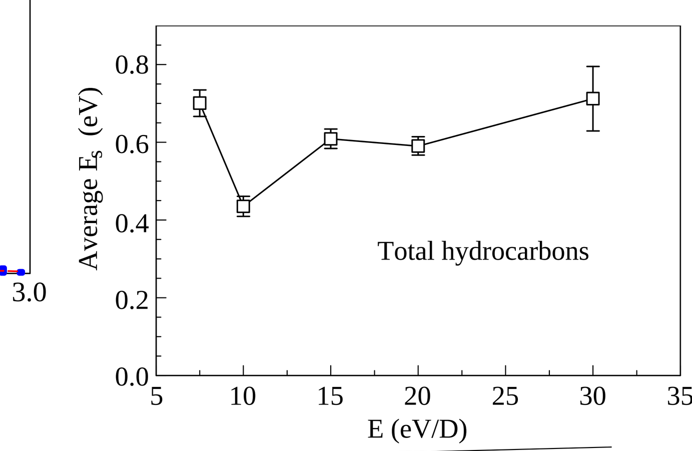


species

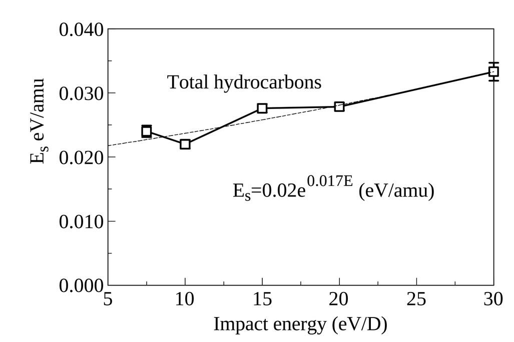


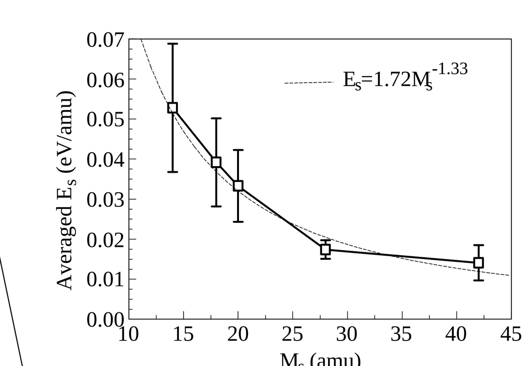


thermalization likely



energy of ejecta



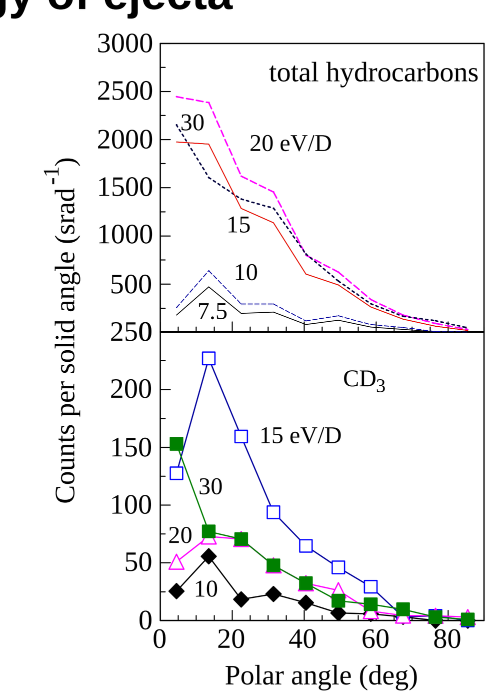


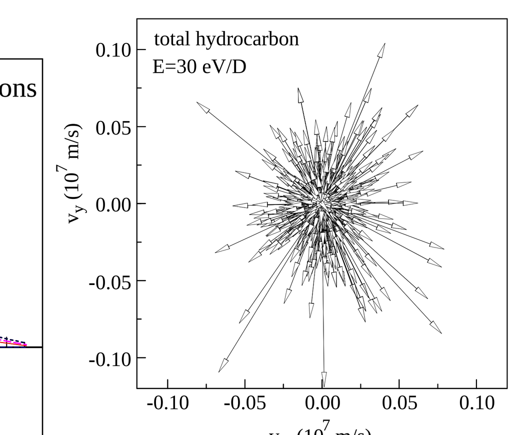
analytical fits

Energy spectra from kinetic desorption
HOT: ~ 5000K

Angular spectra isotropic in the plane of surface

Oriented upward from the surface





angular

References

[1] Brenner et al., *J Phys. Cond. Matt.* **14** 783 (2002).

[2] L. I. Vergara, F. W. Meyer, H. Krause, P. Traskelin, K. Nordlund, and E. Salonen, *J. Nucl. Mat.*, in press (2006).