

Reflection and chemical sputtering spectra at fusion edge plasma facing carbon

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Domain : Fusion

We study interactions of deuterium atoms and vibrationally excited deuterium molecules with deuterated amorphous and crystalline graphite surfaces at a range of low impact energies (5-30 eV/D). Molecular dynamics simulations of this complex system yields reflection spectra of D and D₂, chemically sputtered hydrocarbon and D₂ yields, as well as their energy and angular spectra [1]. Particular attention is paid to preparation of surfaces (by particle irradiation), to internal (rovibrational) state of impinging particles and to the choice of hydrocarbon potentials (REBO [2] and AIREBO [3]). Our data are in good agreement with available experimental results [4,5].

[1] P. S. Krstić, C. O. Reinhold, and S. J. Stuart, *Eurphysics Letters* (2006, submitted).

[2] D. W. Brenner et al., *J. Phys.: Condens. Matter* 14, 783 (2002).

[3] S. J. Stuart et al., *J. Chem. Phys.* 112, 6473 (2000).

[4] L. I. Vergara et al., *J. Nucl. Matls.* 347, 118 (2005).

[5] F. W. Meyer et al., *Phys. Scr.* T124, 44 (2006).