Molecular Dynamics Simulation for Physical Sputtering of Surfaces made of Lennard-Jones Atoms

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Collision cascade dynamics has been widely studied experimentally and theoretically. However, even for particles interacting via simple two-body potential functions such as Lennard-Jones potential functions, the exact dependence of the sputtering yield on the potential functions has not been well understood yet. The goal of this study is to evaluate the sputtering yield of a surface made of particles interacting with Lenard-Jones potential by the injection of energetic particles of fully repulsive interaction. In general, the sputtering yield should be low if the bond energy of the material is strong (so that particles are not easily desorbed from the surface) and it should be high if the collision cross section, i.e., repulsive force at short interatomic distances, is large (so that the incident energetic particle transfers its momentum more efficiently to particles that constitute the substrate). In this study, we study quantitatively how the interatomic potential impacts the sputtering yield, using molecular dynamics (MD) simulations for particles interacting through a Lennard-Jones potential function (i.e., Lennard-Jones atoms).

For this study, two potentials are considered: a “full” LJ potential for the interaction among the substrate particles and a “repulsive” LJ potential for the interaction with the incident particles. The latter is simply the repulsive part of the “full” LJ potential. MD simulations have been performed to evaluate the sputtering yield of Lenard-Jones atoms. The mass and interaction length of the “repulsive” LJ potential of the incident particle are in general set to be different from those of the particles that constitute the substrate. It has been found that the sputtering yield present a strong dependency on these two parameters.