Simulation of the Desorption Process induced by Fast Ionic Atoms, Molecules, or Clusters

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A large Computer Code CLIMPACT has been set up to simulate the Desorption Process induced by fast (keV to MeV per amu) heavy ions, molecules or clusters.

The coupled equations for the Molecular Dynamics for some 10.000 to 100.000 particles are solved for a setup of an array of atoms impinged by a cluster of atoms treated the same way.

The target atoms were assumed to be arranged in an *fcc* crystal structure bound by a two-body Lennard-Jones-type force.

The projectile is allowed to impinge in an arbitrary angle. The trajectories of all particles are followed, showing the forming of a shock wave inside the material, especially if the projectile contains more than one atom (coherent superposition).

Subtle difficulties in such large highly non-equilibrium Molecular Dynamics calculations are given special care.

Boundary conditions at the side of the studied piece of matter should simulate that the piece is just a part of an extended homogenous solid. Thus, e.g. a shock wave should not get reflected at the border of the lattice piece taken. We have proven that this problem can only be solved by introducing **non-local** boundary conditions. We use the simplest version of it adding a friction force to the dynamic equation with its strength and its power-dependence of the velocity dependence determined by studying the case of a linear chain. This force applies to the motion of all atoms within three atomic distances from the boundary layer.

The inherent necessary recognition of next neighbours in each step is done by a grid method which automatically adjusts its size to the momentary occuring relative atom velocities.

Calculations have been performed for a large range of energies, sizes and different angles of the incoming ions. The solid was simulated by a $16 * 16 * 16$ cubic cell bloc.

CLIMPACT is now ready for being applied on a routine basis.