Onset of spallation in solid argon by a shockwave: a molecular dynamics study

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Molecular dynamics simulations of shockwaves in solid argon were performed. The simulation consisted of a orthorhombic cell of 34.2382 Å and 684.764 Å, that contain 17280 atoms at 5K interacting by means a pair potential type[1]. The shockwave (Fig.1) itself was introduced explicitly in the simulation by a piston hitting the sample from one side of the simulation box, at speeds ranging from 1.2 to 1.3 times the speed of sound in solid argon at the chosen density.

In order to characterize the sample in terms of both structural and dynamic properties, we studied the density and temperature profiles, and quantify the particles diffusion.

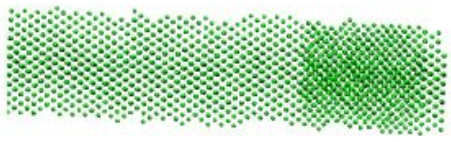

Fig. 1 *The passage of the shockwave across the sample.*

Our simulations reproduce the experimental Hugoniot curve, as well as fracture of the material induced by rarefaction waves. Local melting is seen as the shockwave travels through the sample (according to atomic diffusion and local common neighbor analysis), and evidence is presented for a high–density disordered phase. When the piston stops, a rarefaction wave develops, producing a large tensile stress, which finally causes the failure of the sample by a ductile fracture.

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[1] M. Ross, Phys. Rev. A 8, 1466 (1973)