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Shock and detonation processes studied at the nanoscale[1]

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We report recent advances on shock and detonation processes studied at the nanoscale using several simulation techniques. Concerning shock physics, example of the investigation of spallation phenomena in copper and tantalum using large scale Molecular Dynamics will be given. Concerning High Energetic materials, example of the use of Monte Carlo techniques to build the equation of state (EOS) of nitromethane is shown. Thermodynamic properties of detonation products are computed using Reactive Monte Carlo simulations, including an explicit treatment of carbon clusters based on reactive potential results. Finally, we develop equilibrium methods for the simulation of isentropic processes (either during the compression or the release of a material), that we applied to study the release of a monoatomic liquid. These results are compared to the direct non-equilibrium MD simulations of the same process, showing that the isentropic approximation is not strictly valid.

[1]In collaboration with Emeric Bourasseau, Guillaume Chevrot, Nicolas Desbiens, Nicolas Pineau, and Laurent Soulard, Commissariat à l'Energie Atomique (CEA-DAM).