

Abstract Submitted
for the SHOCK11 Meeting of
The American Physical Society

Mesoscopic simulations of Nitromethane JEAN-BERNARD MAILLET, EMERIC BOURASSEAU, NICOLAS DESBIENS, CEA-DAM, GABRIEL STOLTZ, CERMICS - Ecole de Ponts Paris Tech — We present recent developments of the Dissipative Particle Model that allow simulating the physico-chemical behavior of a molecular material at the mesoscale level. Several ingredients have been added to the previous model (see JB Maillet, L. Soulard and G. Stoltz, Europhys. Lett., **78**, 68001 (2007)), in particular concerning the intermolecular force field and the contributions of the internal degrees of freedom. Multiple steps chemistry is handled through the use of additional degrees of freedom. This model is applied to micron scale simulations of nitromethane, both at equilibrium and under shock conditions.

Jean-Bernard Maillet
CEA-DAM

Date submitted: 10 Feb 2011

Electronic form version 1.4