Abstract Submitted
for the SHOCK09 Meeting of
The American Physical Society

Phase diagram and thermodynamic properties of nanocarbons in detonation conditions from atomistic simulations using the LCBOPII potential NICOLAS PINEAU, GUILLAUME CHEVROT, EMERIC BOURASSEAU, JEAN-BERNARD MAILLET, JAN LOS, ANNALISA FASOLINO — Several earlier studies showed that the detonation of oxygen deficient explosives produces substantial amounts of nanometre-sized carbon residues. The presence of these carbon nanoparticles needs to be accounted for in thermochemical models to obtain accurate estimations of the thermodynamic properties of the detonation products. Thus the determination of the thermodynamic properties of nanocarbons, and in particular of the size-dependence of their phase diagram, is highly desirable for pressure and temperature ranges close to those achieved at the Chapman-Jouguet point. In this communication we will present the carbon phase diagram obtained by Monte Carlo simulations with the LCBOPII potential, an empirical potential for carbon developed by Los et al. which is known to give a good description of bulk carbon phases under high pressure and temperature [1]. In particular we will emphasize on the region of the phase diagram of interest for detonation products (close to the CJ point) and extrapolations of the coexistence lines to the nanometer-sized carbon clusters will be provided using a simple model. Our results will then be compared to the structure and phase transitions of nanocarbons obtained by Molecular Dynamics simulations.

[1] Phys. Rev. B 72, 214102 (2005)

Nicolas Pineau

Date submitted: 06 Feb 2009 Electronic form version 1.4