

Abstract for an Invited Paper
for the SHOCK07 Meeting of
The American Physical Society

Multiphase equation of state of Carbon from first principles simulations and applications to shock wave experiments and design¹

ALFREDO A. CORREA, Lawrence Livermore National Laboratory and Physics Department, University of California at Berkeley

Hydrodynamic and finite element simulations are of primary importance in the current point design of the ignition capsules for fusion at the National Ignition Facility. In particular, nano-structured diamond has been proposed as an ablator material. The reliability of the hydrodynamic results depends critically on the equation of state tables used as input. Ab initio molecular dynamics and electronic structure calculation had become one of the most useful tools to investigate properties of materials. In this talk we present a concrete example showing how ab initio results can be expressed in a way that is useful for hydrodynamics calculations, particularly we show how to build a analytic equation of state for Carbon that involves solid (diamond, BC8) and liquid phases. Strength properties –important to the interpretation of shock wave experiments– can be added to the model using the same theoretical framework.

In collaboration with Lorin Benedict and Eric Schwegler, Lawrence Livermore National Laboratory.

¹This work was performed under the auspices of the U.S. Dept. of Energy at the University of California/Lawrence Livermore National Laboratory under contract no. W-7405-Eng-48