Abstract Submitted
for the SHOCK15 Meeting of
The American Physical Society

A High Pressure-Temperature Density Functional Tight Binding Model for Carbon with Dispersion Corrections[1] CHRIS CANNELLA, NIR GOLDMAN, Lawrence Livermore National Laboratory — Carbyne (e.g., linear chains of sp-bonded carbon) has been the subject of intense research focus due to its presence in astrophysical bodies, as well as its potential for use as a nanoelectronic device and superhard material. In this work, we discuss the formation of carbyne fiber bundles over a nanosecond time scale in laser pulse melting studies, using a previously determined density functional tight binding model for carbon coupled with a new correction for the dispersion energy. We determine our dispersion energy model by optimizing a modified Lennard-Jones potential to an experimentally determined equation of state for graphite, yielding excellent results for the bulk modulus and density under ambient conditions. We then simulate previous experiments by heating graphite to high temperature, followed by expanding the ensuing liquid phase to low density. Our results indicate that the initial, hot liquid phase mainly consists of sp^2-bonded carbon atoms, which form a system of sp-bonded strands bound together via dispersion interactions upon achieving low density and temperature. The high computational efficiency of our approach allows for direct comparison with experiments that span a wide range of thermodynamic conditions, and can help determine parameters for synthesis of carbon-based materials with potentially exotic properties.

[1]This work performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under Contract DE-AC52-07NA27344.

Abstract APS
APS

Date submitted: 16 Jun 2015 Electronic form version 1.4