Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

First Principles Phonon and Elasticity Computations for Iron under extreme conditions[1] XIANWEI SHA, R.E. COHEN, Carnegie Institutiion of Washington — We performed linear-response Linear-Muffin-Tin-Orbital (LMTO) and particle-in-cell (PIC) model calculations to understand and predict the lattice dynamical, thermal equation of state and elastic properties of bcc, fcc, and hcp iron as functions of pressure and temperature. The phonon dispersion and phonon density of states have been calculated at different volumes and show good agreement with experiment. We derived the Helmholtz free energy based on both the linear response LMTO and PIC calculations, and found that the calculated geometric mean phonon frequencies and free energies from these two different methods agree well under pressure, in contradiction to an earlier calculation. We performed detailed investigations on the behavior of elastic constants and various thermal equation of state parameters, including the bulk modulus, the thermal expansion coefficient, the Grüneisen ratio, and the heat capacity as functions of temperature and pressure. We made detailed comparison with experiment and earlier theoretical calculations. We do not find the large change in c/a axial change with T. Sound velocities at extreme conditions have also been examined. These first-principles data provide important information to understand shock dynamics and other interesting phenomena under extreme conditions.

[1]This work was supported by US Department of Energy ASCI/ASAP subcontract to Caltech, Grant DOE W-7405-ENG-48 (to REC).

Xianwei Sha
carnegie Institutiion of Washington

Date submitted: 22 Dec 2005 Electronic form version 1.4