Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Multi-scale modeling of ferromagnetism in bcc Fe as a function of pressure and temperature XIANWEI SHA, R. E. COHEN, Carnegie Institution of Washington — We investigate the magnetic properties of bcc Fe as functions of pressure and temperature using multi-scale modeling techniques. We employ a first-principles fitted tight-binding total-energy model in the generalized-gradient approximation to examine bcc Fe at numerous ferromagnetic, antiferromagnetic and spin spiral states, and fit the tight-binding data to a generalized Heisenberg Hamiltonian which includes both the on-site and local exchange energy to describe the magnetic energy for any arbitrary magnetic configuration. We obtain the Curie temperature, magnetization curve, and other finite-temperature magnetic properties through extensive Monte Carlo simulations, which have been further applied to examine the influence of the magnetic fluctuations on the free energy and thermal equation of state properties of bcc Fe at high temperatures. 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 Institution of Washington

Date submitted: 20 Nov 2006 Electronic form version 1.4