Abstract Submitted
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Thermal equation of state of bcc and hcp Fe: linear response quasi-harmonic lattice dynamics[1] XIANWEI SHA, R. E. COHEN, Geophysical Laboratory, Carnegie Institution of Washington, Washington, DC 20015 — Linear-response Linear-Muffin-Tin-Orbital calculations have been performed to understand and predict the thermal equation of state, elasticity, and phase stability of bcc and hcp Fe, for input into dynamic shock finite-element simulations. The phonon dispersion and phonon density of states have been calculated at different volumes and various c/a axial ratios for hcp structures, which show good agreements with available experimental data. The thermal conductivity and electrical resistivity at different pressure have been calculated. Free energy functional for bcc and hcp Fe has been derived, and has been further applied to establish the thermal equation of state, bulk modulus K_0, dK_0/dT, and thermal expansion coefficients under high pressures and temperatures. A detailed comparison with experiment has been made. For hcp Fe, the variations of c/a ratios with temperatures and pressures have been predicted. The influence of anharmonic effects has been examined using tight-binding calculations. This work was supported by US Department of Energy ASCI/ASAP subcontract to Caltech , Grant DOE W-7405-ENG-48 (to REC).

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