Simulating Iron at the Pressures and Temperatures of the Earth’s Core

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The melting curve of iron at the conditions of the Earth’s core is still ambiguous by about 1000 K. In order to predict the properties of Fe at high pressures and temperatures, we have developed a reactive force field based on bond length/bond strength relationships. The force field was fitted to first-principles-derived energy versus volume curves, focusing on pressures of the core (135-360 GPa) for iron in various structures: hcp, bcc, fcc, sc, and diamond (a4). We also included vacancy energies for fcc and sc. We conducted two types of molecular dynamics simulations in order to obtain high-temperature, high-pressure properties of Fe. First we ran single-phase NPT heating and cooling, for 256-atom systems at 5 pressures (150, 200, 250, 300, and 350 GPa) for several heating and cooling rates. We noted a hysteresis in the melting temperature, due to superheating and supercooling effects. Additionally, we found the re-crystallized structures resulting from our cool-down simulations to contain stacking faults – upon reheating, such structures had lower melting temperatures, with an effect similar to a first-time melting run with five vacancies. We also computed the melting curve by solving the Clausius-Clapeyron equation, relating the differences in volume and enthalpy, in the region of hysteresis, to the pressure and temperature. Our results show good agreement with the higher of the published melting curves (Brown and McQueen 1987, Alfe et al. 2002, Nguyen et al. 2004). Second, we use a velocity autocorrelation method along with a hard-sphere model for gas (Lin et al. 2003), to estimate thermodynamic properties (density of states, free energy, entropy, and diffusion) of solid and liquid structures under various pressure and temperature conditions. The computed densities of states display reasonable characteristics for both solid and liquid structures. The entropy differences between liquid and solid are on the order of typical entropies of fusion (~R). While further investigation is warranted, the velocity autocorrelation method should serve as a powerful tool for analyzing the thermodynamic properties of iron at extreme conditions.