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**Ab Initio $\alpha \rightarrow \epsilon$ Transition Barrier in Shocked Iron**[1] MICHAEL P. SURH, BABAK SADIGH, Lawrence Livermore National Laboratory — An ab initio study is presented of the $\alpha \rightarrow \epsilon$-like transition in single crystal iron under uniaxial strain (Kalantar, et. al., Phys. Rev. Lett. 95 075502 (2005)). First-principles ground state DFT calculations for ordered-spin phases predict a magnetostructural transition from ferromagnetic (FM) to an antiferromagnetic (AFM) phase at a uniaxial strain similar to experiment. However, the calculated stress is higher than is inferred from the shock. DFT also predicts a significant energy barrier for the expected atomic shuffle transition from bcc to hcp. In contrast, the experimental kinetics are consistent with a barrier-free or small-barrier transformation path. It is possible that the neglect of thermal spin disorder in the DFT calculations explains these discrepancies. To study this, the spin and atomic order are artificially separated, assuming that the atomic motion is adiabatic on spin time-scales. A Heisenberg-like Hamiltonian is fit to DFT energies of different ordered magnetic phases, and magnetic free energies are calculated for fixed atomic coordinates by Monte Carlo methods. This model predicts a significantly smaller elastic constant than DFT for the FM ground state, and it reduces the transition energy barrier versus ground state values.

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