Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Spin-lattice coupling in BCC iron JUNQI YIN, MARKUS EISENBACH, DON NICHOLSON, Oak Ridge National Laboratory — For empirical iron potentials, the magnetic contribution is usually implicitly considered, and the spin-lattice coupling is simply neglected. From first principle calculations, we proposed a Heisenberg type of exchange for BCC iron that couples the spin and lattice degrees of freedom. The parameterization is based on quantities already employed in embedded-atom potentials. Therefore, the model is a natural augmentation of the existing iron potentials, and is applicable to molecular dynamics simulations. Our model built on Dudarev potential can reproduce iron's specific heat from the Curie temperature down to about 400K, and the estimate of the spin-lattice contribution indicates that it is significant near the transition. We applied our model to studying a $< 111 >$ screw dislocation in BCC iron, and found evidences that the dislocation core has a local transition temperature different from the bulk one. Work is sponsored by the U.S. DOE, Office of Basic Energy Sciences, Materials Sciences and Engineering Division (M. E., D. M. N.), and by Office of Advanced Scientific Computing Research (J. Y.). This research used resources of the Oak Ridge Leadership Computing Facility at the ORNL, which is supported by the Office of Science of the U.S. DOE under Contract No. DE-AC05-00OR22725.

Junqi Yin
Oak Ridge National Laboratory

Date submitted: 27 Nov 2012 Electronic form version 1.4