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Effect of lattice vibrations on magnetic phase transition in BCC Iron JUNQI YIN, MARKUS EISENBACH, AURELIAN RUSANU, DON NICHOLSON, Oak Ridge National Lab — From the first principle calculation of BCC iron, we build a classical Heisenberg model with the interaction coupling as a function of both the distance and local environments(e.g. volume). Using the Johnson potential and Finnis-Sinclair potential, we perform Monte Carlo simulations of BCC iron including the effect of lattice vibrations. The validity of classical Heisenberg model in describing the magnetic phase transition of BCC iron is explained.

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