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Finite Temperature Lattice Vibrations and the Magnetic Structure of Fe and Ni[1] G. MALCOLM STOCKS, Oak Ridge National Laboratory, YANG WANG, Pittsburgh SuperComputer Center, ROGER STOLLER, Oak Ridge National Lab., AURELIAN RUSANU, University of Tennessee, MARKUS EISENBACH, DONALD NICHOLSON, GERMAN SAMOLYUK, Oak Ridge National Lab. — Modern *ab initio* theories of the magnetic phase transition (Curie Temperature, T_C) of Fe and Ni based on the Disordered Local Moment (DLM) type models generally rely on (constrained) density functional theory calculations performed at 0K and assume that the atoms occupy their equilibrium lattice sites. Here we point out that finite temperature lattice vibrations can result in large fluctuations in the local moments associated with individual site beyond those already accounted for in these approaches. These conclusions are based on large cell ($\sim 10^4$ – atoms) *ab initio* calculations of the magnetic state of Fe and Ni based on the O[N] Locally Self-consistent Multiple Scattering (LSMS) method. Atom positions are obtained from freezes of individual time steps of molecular dynamics simulations based on classical interaction potentials. Calculations are performed for a range of temperatures up and beyond T_C that illustrate the extent of the moment fluctuations. We discuss the consequences of these findings for the adequacy of existing theories T_C.

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