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Combined Molecular Dynamics-Spin Dynamics Simulation of α-Iron in an External Magnetic Field MARK MUDRICK, DILINA PERERA, DAVID P. LANDAU, Univ of Georgia — Using an atomistic model that treats both translational and spin degrees of freedom, combined molecular and spin dynamics simulations have been performed to study dynamic properties of α-iron. Atomic interactions are described by an empirical many-body potential[1] while spin-spin interactions are handled with a Heisenberg-like Hamiltonian with a coordinate dependent exchange interaction[2]. Each of these interactions are parameterized by first-principles calculations. These simulations numerically solve equations of motion using an algorithm based on the second-order Suzuki-Trotter decomposition for the time evolution operator[3]. Through calculation of the Fourier transform of space-displaced time-displaced correlation functions, vibrational and magnetic excitations have been studied. The application of an external magnetic field up to 10-T has now been included and has been shown to increase the characteristic frequencies of the single-spin-wave excitations. Two-spin-wave interactions have also been investigated.

[1]Dudarev S L, Derlet P M 2005 *J. Phys.: Cond. Matter* **17** 7097
[2]Ma P W, Woo C H, Dudarev S L 2008 *Phys. Rev. B* **78** 024434
[3]Perera D, et al. 2014 *J. Phys.: Conf. Ser.* **487** 012007

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