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Combined Molecular and Spin Dynamics Simulation of Lattice Vacancies in BCC Iron[1] MARK MUDRICK, Univ of Georgia, DILINA PERERA, Mississippi St Univ, MARKUS EISENBACH, Oak Ridge National Laboratory, DAVID P. LANDAU, Univ of Georgia — Using an atomistic model that treats translational and spin degrees of freedom equally, combined molecular and spin dynamics simulations have been performed to study dynamic properties of BCC iron at varying levels of defect impurity. Atomic interactions are described by an empirical many-body potential[2], and spin interactions with a Heisenberg-like Hamiltonian with a coordinate dependent exchange interaction[3]. Equations of motion are solved numerically using the second-order Suzuki-Trotter decomposition for the time evolution operator[4]. We analyze the spatial and temporal correlation functions for atomic displacements and magnetic order to obtain the effect of vacancy defects on the phonon and magnon excitations. We show that vacancy clusters in the material cause splitting of the characteristic transverse spin-wave excitations, indicating the production of additional excitation modes. Additionally, we investigate the coupling of the atomic and magnetic modes. These modes become more distinct with increasing vacancy cluster size.

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[4]Perera D, et al. 2014 *J. Phys.: Conf. Ser.* **487** 012007

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