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Molecular dynamics, spin dynamics study of phonon-magnon interactions in BCC iron[1] DILINA PERERA, DAVID P. LANDAU, Center for Simulational Physics, The University of Georgia, G. MALCOLM STOCKS, DON NICHOLSON, MARKUS EISENBACH, JUNQI YIN, Oak Ridge National Laboratory — By combining an atomistic many-body potential (Finnis-Sinclair) with a classical Heisenberg-like spin Hamiltonian, we perform combined molecular and spin dynamics simulations to investigate phonon-magnon interactions in BCC iron. The coupling between atomic and spin degrees of freedom is established via a distance dependent exchange interaction derived from first principles electronic structure calculations. Coupled equations of motion are integrated using a second order Suzuki-Trotter decomposition of the exponential time evolution operator. To investigate the effect of lattice vibrations on spin wave spectrum, we calculate spin-spin and density-density dynamic structure factors S(q, ω), and compare that to the results obtained from pure spin dynamics simulations performed on a rigid lattice. In the presence of lattice vibrations, we observe an additional peak in the longitudinal spin-spin dynamic structure factor which coincides with the peak position in density-density dynanmic structure factor.

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Dilina Perera
Center for Simulational Physics, The University of Georgia

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