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Spin-orbit induced relaxation in combined molecular and spin dynamics simulations of BCC iron[1] DILINA PERERA, The University of Georgia, MARKUS EISENBACH, Oak Ridge National Laboratory, DON NICHOLSON, University of North Carolina at Asheville, JUNQI YIN, University of Tennessee, G. MALCOLM STOCKS, Oak Ridge National Laboratory, DAVID P. LANDAU, The University of Georgia — The combined molecular and spin dynamics (MD-SD) method has emerged as a powerful tool for integrating the effect of magnetism into the atomistic simulations of transition metals. The coupling between the atomic and spin degrees of freedom is established via a coordinate-dependent exchange interaction, which allows the dynamic exchange of energy between the lattice and spin subsystems; however such exchange-based coupling alone cannot facilitate the transfer of angular momentum between the two subsystems. This results in an unrealistic depiction of the spin-lattice relaxation process. To circumvent this drawback, we extend the conventional MD-SD approach by incorporating additional interaction terms that characterize spin-orbit coupling. These interactions are modeled in terms of the local magnetic anisotropies that arise as a consequence of the symmetry breaking due to lattice vibrations. Using MD-SD simulations, we investigate the effect of these terms on the spin-lattice relaxation in BCC iron. By coupling a conventional thermostat to the lattice subsystem, we show that this novel extension enables the exchange of angular momentum and leads to the mutual thermalization of both lattice and spin subsystems.

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