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Spin-lattice Dynamics Simulation: Method and Applications

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Abstract

Applications involving materials properties governed by the magnetic nature of electron spin are quickly becoming an essential ingredient in the more advanced technologies in many important areas of engineering. The main challenge in the modeling of the dynamics process of magnetic materials is to associate their structural and mechanical properties to magnetism. We developed a model to treat magnetic atoms as classical particles with intrinsic spins. They interact via scalar many-body forces as well as via spin-orientation-dependent forces. The strength of the interaction between atoms becomes depending on the relative collinearity of their spins. Algorithm for the integration of equations of motion, parallel programming algorithm and the spin thermostat are introduced. We investigated several applications of the method. The isothermal magnetization curve evaluated using the spin-lattice dynamics algorithm is well described by the mean-field approximation and agrees satisfactorily with the experimental data for a broad range of temperatures. The equilibrium time-correlation functions of spin orientations exhibit the presence of short-range magnetic order above the Curie temperature. Short-range order spin fluctuations are shown to contribute to the thermal expansion of the material. Simulations on thermal expansion and elastic response of bulk bcc iron, and magnetization in iron thin films are also performed. Our analysis illustrates the significant part played by the spin directional degrees of freedom in the dynamics of atomic motion in magnetic iron and iron-based alloys, and shows that the spin-lattice dynamics algorithm provides a viable way of performing realistic large-scale dynamical simulations of magnetic materials.

About the Speaker

Pui Wai Ma received his Ph.D. degree in the Department of Electronic and Information Engineering of The Hong Kong Polytechnic University, and his M.Phil. and B.Sc. degree in the Department of Physics of The University of Hong Kong. He is now working with Prof. C. H. Woo on the modeling of ferromagnetic materials, especially on the computer simulation of magnetic metals.

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