DYNAMICS OF DILUTED MAGNETIC SEMICONDUCTORS FROM ATOMISTIC SPIN DYNAMICS SIMULATIONS

J. Hellsvik[1], B. Skubic[1], L. Nordström[1], B. Sanyal[1], P. Nordblad[2], P. Svedlindh[2], O. Eriksson[1]

[1]*Department of Physics and Materials Science, Uppsala University, Sweden*
[2]*Department of Engineering Science, Uppsala University, Sweden*

A computational scheme, Atomistic Spin Dynamics (ASD), based on density functional theory, the adiabatic approximation and the atomic moment approximation is presented. The present implementation of the method incorporates a parametrization of the magnetic exchange interactions to a classical Heisenberg Hamiltonian. With simulation cells containing up to 100 000 local magnetic moments, this approximation allows for studies of the magnetization dynamics for time intervals exceeding 100s of picoseconds.

Dilute magnetic semiconductors continue to attract attention, motivated primarily by their possible applications to spintronics. They are also interesting per se as manifestations of magnetic systems with complex geometries. The time evolution of pair correlation and autocorrelation functions has been studied with ASD simulations of the dilute magnetic semiconductor, Mn-doped GaAs. The dynamics of this DMS system reveal a substantial short ranged magnetic order even at temperatures at or above the ordering temperature, with a non-vanishing pair correlation function extending up to several atomic shells. For the high As antisite concentrations the simulations show a short ranged anti-ferromagnetic coupling, and a weakened long ranged ferromagnetic coupling. For sufficiently large concentrations we do not observe any long ranged ferromagnetic correlation. A typical dynamical response shows that starting from a random orientation of moments, the spin-correlation develops very fast (~1ps) extending up to 15 atomic shells. Above ~10 ps in the simulations, the pair correlation is observed to extend over some 40 atomic shells. The autocorrelation function has been calculated and compared with ferromagnets like bcc Fe and spin glass materials.