Atomistic simulations of the magnetic neutron scattering from nanoparticles along the hysteresis loop: effects of surface anisotropy

Michael P. Adams[1], Andreas Michels[1], Hamid Kachkachi[2]

[1]*Department of Physics and Materials Science, University of Luxembourg, 162A avenue de la Faiencerie, L-1511 Luxembourg, Grand Duchy of Luxembourg*

[2]*Universite de Perpignan via Domitia, Laboratoire PROMES CNRS UPR8521, Rambla de la Thermodynamique, Tecnosud, F-66100 Perpignan, France*

Michael P. Adams, michael.adams@uni.lu

We consider a dilute ensemble of randomly-oriented spherical nanomagnets and investigate its magnetization structure and ensuing neutron-scattering response by numerically solving the Landau-Lifshitz equation. Taking into account the isotropic exchange interaction, a cubic magnetic core anisotropy, an external magnetic field, and in particular the Néel surface anisotropy, we compute the magnetic neutron scattering cross section and pair-distance distribution function from the obtained equilibrium spin structures. The numerical results are compared to the well-known analytical expressions for uniformly magnetized particles and provide guidance to the experimentalist. Moreover, the (directed) Néel surface anisotropy is compared to a random surface anisotropy, and the effect of a particle-size distribution function is modeled. The following figure illustrates some of our simulation results for the magnetic neutron scattering cross section of spherical nanoparticles with different types of surface anisotropy.

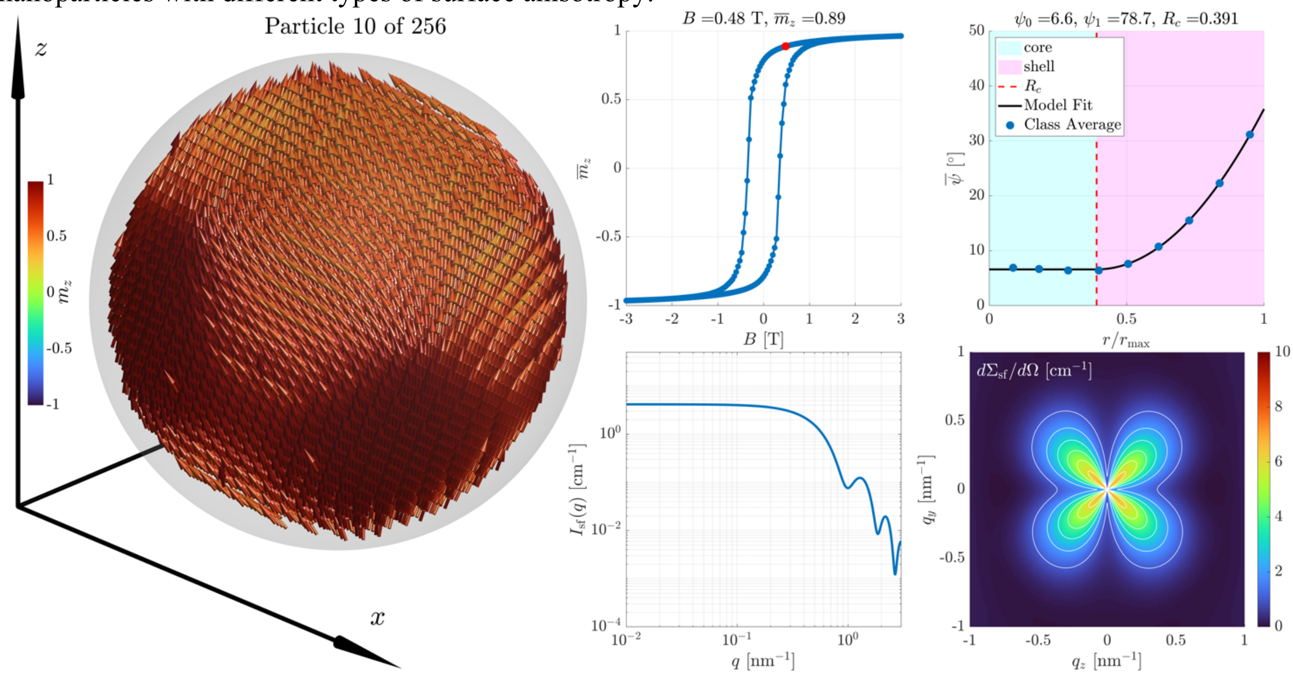

Figure 1: Simulation results (snapshot) of a dilute ensemble of 256 spherical nanoparticles (diameter: 8 nm) with tangential Néel surface anisotropy and corresponding spin-flip neutron scattering cross section along the hysteresis loop. The function $\overline{\psi}$ is a measure for local spin deviations from the macrospin state, that allows to distinguish between ferromagnetic core and non-ferromagnetic shell domains, where the transition radius R_c is a field dependent quantity.

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