Signature of surface anisotropy in the spin-flip neutron scattering cross section of spherical nanoparticles: Atomistic simulations and analytical theory

M. P. Adams[a], E. P. Sinaga[a], H. Kachkachi[b], and A. Michels[a]
[a]*Department of Physics and Materials Science, University of Luxembourg, 162A Avenue de la Faiencerie, L-1511 Luxembourg, Grand Duchy of Luxembourg*
[b]*Université de Perpignan via Domitia, Laboratoire PROMES CNRS UPR8521, Rambla de la Thermodynamique, Tecnosud, F-66100 Perpignan, France*

We investigate the signature of magnetic surface anisotropy in nanoparticles in their spin-flip neutron scattering cross section. Taking into account the isotropic exchange interaction, an external magnetic field, a uniaxial or cubic magnetic anisotropy for the particle's core, and several models for the surface anisotropy (Néel, conventional, random), we compute the spin-flip small-angle neutron scattering (SANS) cross section from the equilibrium spin structures obtained using the Landau-Lifshitz equation. The sign of the surface anisotropy constant, which is related to the appearance of tangential- or radial-like spin textures, can be distinguished from the momentum-transfer dependence of the spin-flip signal. The data cannot be described by the well-known and often-used analytical expressions for uniformly magnetized spherical or core-shell particles, in particular at remanence or at the coercive field. Based on a second-order polynomial expansion for the magnetization vector field, we develop a novel minimal model for the azimuthally averaged magnetic SANS cross section. The theoretical expression considers a general magnetization inhomogeneity and is not restricted to the presence of surface anisotropy. It is shown that the model describes very well our simulation data as well as more complex spin patterns such as vortexlike structures. Only seven expansion coefficients and some basis functions are sufficient to describe the scattering behavior of a very large number of atomic spins.

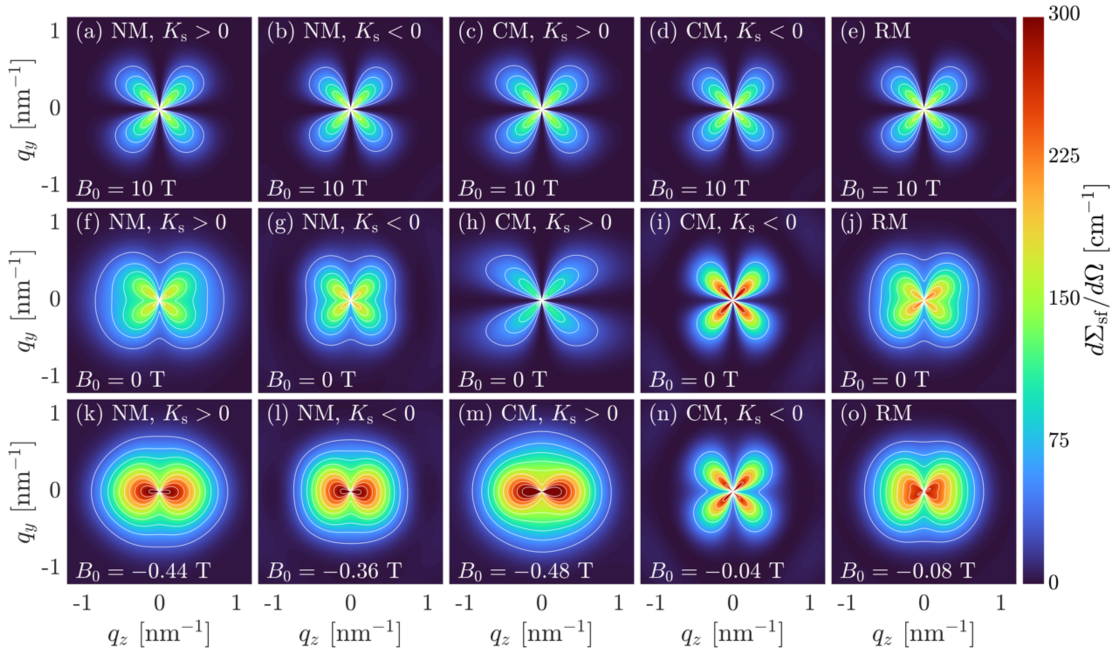

Figure 1: Spin-Flip SANS cross sections for nanoparticles with different surface anisotropies [1].

References

[1] M. P. Adams *et al.*, Phys. Rev. B **109**, 024429 (2024).

Submitting Author: michael.adams@uni.lu