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Micromagnetic simulation of neutron scattering from spherical nanoparticles: Effect of pore-type defects

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It is well known that beyond a certain size magnetic nanoparticles exhibit a nonuniform internal spin structure. This feature, which is of relevance for many problems of practical interest (e.g., biomedical imaging and drug delivery), is commonly ignored when it comes to the analysis of magnetic neutron scattering data on nanoparticle ensembles. By means of numerical micromagnetic computations we study the transition from single-domain to multi-domain behavior in nanoparticles and its implications for the ensuing elastic magnetic small-angle neutron scattering (SANS) cross section. Furthermore, we model the effect of pore-type microstructural defects on the magnetic SANS cross section and the related pair-distance distribution function of spherical magnetic nanoparticles. Our expression for the magnetic energy considers the isotropic exchange interaction, the magneto-crystalline anisotropy, the dipolar interaction, and an externally applied magnetic field. The signatures of the defects and the role of the dipolar energy are highlighted, and the effect of a particle-size distribution is studied. We are also interested in the signature of the Dzyaloshinskii-Moriya interaction on the SANS observables.

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