A reverse Monte Carlo algorithm to simulate two-dimensional small-angle scattering intensities

L. C. Barnsley¹, N. Nandakumaran², A. Feoktystov³, M. Dulle⁴, L. Fruhner⁴, M. Feygenson⁵, ⁴

1. Australian Synchrotron, ANSTO, Clayton 3168, Australia, 2. Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-2) and Peter Grünberg Institut (PGI), JARA-FIT, 52425 Jülich, Germany, 3. Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS) at Heinz Maier-Leibnitz Zentrum (MLZ), 85748 Garching, Germany, 4. Forschungszentrum Jülich GmbH, Jülich Centre for Neutron Science (JCNS-1), 52425 Jülich, Germany, 5. European Spallation Source ERIC, SE-22100, Lund, Sweden

Email of communicating author lester.barnsley@ansto.gov.au

Keywords: small-angle scattering; magnetic nanoparticles, reverse Monte Carlo simulations

Small-angle neutron scattering (SANS) and small-angle X-ray scattering (SAXS) are important, experimental techniques for studying the behaviour and properties of materials on the nanoscale. Small-angle scattering (SAS) has been used to investigate systems relevant to a range of scientific fields, including polymers [1], inorganic nanoparticles [2] and magnetic vortices [3]. While the technique is well-established for its versatility and compatibility with a range of sample environments for in-situ studies, analysis of experimentally acquired data is still challenging, particularly in light of the growing complexity of the studied systems.

Numerous out-of-the-box options exist for analysing structures measured by SAS, but many of these are underpinned by assumptions about the underlying interactions that are not always relevant for a given system. In this presentation, we describe a numerical algorithm based on reverse Monte Carlo simulations to model the intensity observed on a SAS detector as a function of the scattering vector [4]. The model simulates a two-dimensional detector image, accounting for magnetic scattering, instrument resolution, particle polydispersity and particle collisions, while making no further assumptions about the underlying particle interactions.

By simulating a 2-D image that can be potentially anisotropic, the algorithm is particularly useful for studying systems driven by anisotropic interactions. The final output of the algorithm is a relative particle distribution, allowing visualisation of particle structures that form over long-range length-scales (i.e., several hundred nanometres), along with an orientational distribution of magnetic moments. We show the effectiveness of the algorithm by modelling a SAS experimental dataset studying finite-length chains consisting of magnetic nanoparticles, which assembled in the presence of a strong magnetic field due to dipole interactions [5].

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