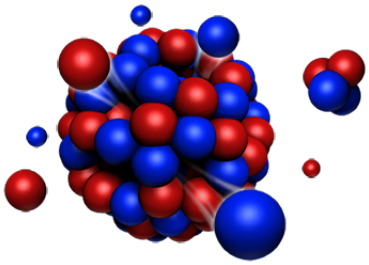

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Challenges for Grazing Incidence Neutron Scattering at Pulsed Sources: Beyond basic experiments and data analysis

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Conventional analysis of reflectometry data provides only structural parameters via fitting model to the data. Can we obtain access to the interaction parameters causing this structure? To realize this one needs a different approach to the data analysis, that includes development of computational workflow capable of generating theoretical models in quantitative agreement with the data.
Grazing Incidence Neutron Scattering experiments simultaneously measure specular reflection, off-specular scattering (OSS) and grazing incidence small angle scattering (GISANS) and deliver the most exhaustive and detailed information on the 3-dimensional structure of thin films and hidden interfaces on enormous length scale.
At present, most of published data in reflectometry are obtained with specular reflectivity, from which the structural information perpendicular to the sample surface is obtained along the Qz component of the wave vector transfer. However, functionality often arises at the mesoscale, where defects, interfaces, and non-equilibrium structures are formed [1], which cannot be resolved only by specular reflectivity alone.
Spallation neutron sources deliver outstanding experimental conditions to perform simultaneously a combined measurement of specular reflection, OSS and GISANS using time-of-flight (TOF) [2]. GINS pilot experiments performed at the SNS on the Magnetism Reflectometer [2] on a multilayer heterostructure of magnetic nanoparticles self-assembled in a block-copolymer matrix will be presented.

Thus, a combination of GINS experiments with the computational workflow capable of generating theoretical models in quantitative agreement with experimental data establishes a direct and precise correlation between local interfacial characteristics and global physical properties. The first results on the implementation of a computational workflow integrating high performance computing (HPC) with GINS experiment via an intuitive, cross-platform user interface is being developed at SNS/ORNL and will be presented [3].

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[1] From Quanta to the Continuum: Opportunities for Mesoscale Science, a report from the Basic Energy Sciences Advisory Committee (2012)
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[2] V. Lauter, H.J.C. Lauter, A. Glavic, B. Toperverg, book chapter in Reference Module Material Science Elsevier, 2016
[3] Mahalik J.P., Dugger J.W., Sides S.W., Sumpter B.G., Lauter V.V., Kumar R., "Interpreting Neutron Reflectivity Profiles of Diblock Copolymer Nanocomposite Thin Films Using Hybrid Particle-Field Simulations", Macromolecules, 51, 8, 3116–3125 (2018)

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