canSAS-VIII, Apr. 14-16, J-PARC, Tokai, Japan

# Information Content, Error Propagation and Systematics

R. P. Hjelm[1]
[1]Lujan Neutron Scattering Center, Los Alamos, NM
E-mail:

Inference on nanoscale structure and the confidence that can be placed on the result is a little explored area, but is of critical concern in forwarding the potential of the small-angle scattering (SAS) technique. Within the vignette of the measurement, over length scales from sub nm to *ca* 10 μm, the data is incomplete and subject to uncertainties in both intensity and momentum transfer. More fundamentally, however, is the classic uniqueness problem, as the phase information needed to construct an image of the structure is missing in the scattering measurement that registers only intensity. Techniques have been developed over the past few decades to address the later problem through neutron isotope labeling techniques and contrast variation in small-angle neutron scattering (SANS) and co-fits of SAXS and SANS data. These mature methods have proven to be very powerful for the solution of structures involving particles of sizes within the measurement domain of SAS. Important examples include bio-structures, colloids, polymers and nanoparticles.

Newer challenges are emerging in areas such as metallurgy, ceramics and geomaterials. These areas have traditionally relied on diffraction for structural studies over atomistic length scales. More recently there has been a realization that nanoscale phase segregation, voids, pores and cracks in these materials are important in understanding the connections between structure, properties and performance. These features are accessible to SAS which can provide unique information. However, there is usually little latitude in experimental design to remove the ambiguity inherent in data interpretation and modeling; thus, to address the large scale structures of these materials there is a pressing need to develop techniques that combine information from SAS measurements with that from other techniques.

In this introduction I will review the data assessment, analysis and inference methods currently in use, with an emphasis on how these methods advance analysis techniques for SAS. I will present remarks to focus the ensuing discussions on how these techniques address the problem of removing modeling ambiguities through an analysis of SAS information content with emphasis of combining SAS data with other characterization methods using Baysian inference and neural network analysis.