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Invited Lecture

Metadata for Small-Angle Scattering Measurements

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Measurements based on small-angle scattering (SAS) of X-rays or neutrons (SAXS or SANS) differ critically in several ways from those based on X-ray or neutron Bragg diffraction (XRD or ND) or on X-ray or neutron spectroscopic methods. XRD or ND measurements yield diffraction peaks at discrete scattering angles or scattering vectors, Q , from which a pattern may be identified, and from there the underlying crystal structure. Similarly, spectroscopic measurements frequently yield information directly relatable to bond energies or energies of transition within the sample material. In contrast, SAXS or SANS measurements yield data that usually comprise a smooth curve of SAS intensity as a function of scattering angle or Q . This requires interpretation in terms of the likely scattering features (inhomogeneities) that underlie the sample microstructure before a quantifiable data analysis can be carried out in any meaningful way. Thus, in archiving SAXS or SANS data, very significant emphasis is required on the metadata to accompany the measured data – both metadata providing detailed qualitative information on sample microstructures, and metadata providing detailed instrumental parameters and other information on the measurements, themselves.

Metadata requirements for SAS are inextricably linked to aspects that may be more-or-less closely related to the measurements, themselves. Examples might include the measurement configuration (SAXS *versus* SANS, transmission *versus* grazing-incidence geometry, 1D Bonse-Hart *versus* 2D pinhole camera, angular-dispersive SAXS or SANS *versus* time-of-flight SANS, etc.), the nature of the sample (e.g., precipitates in metallic alloys, pores in ceramics, polymer structures, nanoparticles in suspension, protein complexes, expected polydispersity in feature size and shape, etc.), absolute calibration and correction issues (e.g. for scattering geometry and Q -values, scattering intensity, effective sample volume), the effective spatial and Q -resolution, background subtraction issues, and even the requirements for common data formats and publication standards. This paper will discuss these issues and current ongoing international efforts within the SAS community to address them.