LCST type phase separation, is known to have a large salt effect. In this study, we selected sodium tetraphenylborate ($NaBPh_4$), whose affinities of anion and cation with water are largely different, as a salt because the solvation effect should be intensive and the formation of large clusters is expected theoretically. In cases of the lower amount of $NaBPh_4$ and water-rich concentration, the mixture becomes colored in blue, and changes to orange with approaching critical temperature. This result suggests that a periodic structure is formed, and its repeat distance increases with increasing temperature. In order to verify the structural formation, we performed SANS measurement at SANS-U in JAEA, Tokai, for the mixtures with 100 mM $NaBPh_4$. The results showed that the profiles have a peak around Q =0.1 A^{-1}, and the peak position shifts to lower-Q with increasing temperature. (K. Sadakane et al., J. Phys. Soc. Jpn. 76, 113602 (2007).) Adding ionic surfactant, for example AOT or SDS, also shows the structural formation as the case of $NaBPh_4$.

Keywords: solvation effect, critical phenomena, periodic structure

P12.07.22

Concentration dependence of static and dynamic structure in a spherical microemulsion system

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The concentration dependence of static and dynamic structure in a microemulsion system has been investigated using the contrast variation small-angle neutron scattering (SANS) and neutron spin echo (NSE) techniques. Since structure factor should not depend on the scattering contrast of systems, a relative form factor is defined as the ratio of the scattering intensities for the different scattering contrasts, which is the ratio of the form factors for the different scattering contrasts. This concept allows us to extract concentration dependence of the shape of the unit particles and the interaction between particles [1]. Furthermore, this strategy is extended to the contrast variation NSE data analyses. The shape and structure fluctuations are successfully decoupled using the relative intermediate form factor method in a droplet microemulsion system [2]. The mean radius of the droplets is almost constant below the droplet concentration, f, of 0.6, while the polydispersity of the system decreases with increasing f. The frequency and the amplitude of the shape fluctuation mode of the droplets increase with f. A collision driven enhancement of the shape fluctuation mode in the high droplet concentration is one of the possible explanations of the dynamics. The attractive interaction between droplets decreases with increasing f below f=0.3, while it increases with f above f=0.3. This suggests that at least two different mechanisms of the change of interaction between droplets exist. Due to the inter-droplet interaction, a clear dynamic slowing down is observed at the length scale corresponding to the inter-droplet distance.

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Keywords: small-angle neutron scattering, neutron spin echo, microemulsion

P12.07.23

Correlation functions of three-phase samples with a film-like or a thread-like phase

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The correlation function of isotropic samples made up of three homogeneous phases is a linear combination of the autocorrelation functions (CF) of the constituting phases. Each of these CFs, referred to as volume CFs (vCF), is the angular average of the overlap volume of a phase with the same phase translated by r. If the thickness of one phase can be assumed negligible the corresponding CF becomes that of a film or a collection of closed films. The resulting autocorrelation function, referred to as film CF (fCF), has an integral expression that involves the only surface(s). Its expression differs from that of the second derivative of a vCF because its integrand no longer contains the two scalar products between the direction of the translation and the normals to the surface at the points separated by r. The first important implication of this result is that fCFs go as 1/r as r goes to zero and, consequently, their contribution to the asymptotic behaviour of small-angle scattering intensities decreases as $1/q^2$ instead of $1/q^4$. The second implication is that the integral expression makes the calculation of the fCF relevant to a monodisperse collection of film-particles shaped as spheres, ellipsoids, cubes or cylinders rather straightforward. In the same way, if one phase extends along a curve and its dimensions transverse to the curve are small, the corresponding limit of the vCF defines the CF of a thread or a collection of threads and its integral expression involves the only curves that define the threads. These CFs go as $1/r^2$ as r goes to zero and contribute to the asymptotic scattering intensities with a term decreasing as 1/q.

Keywords: SAS, micelles microemulsions, helical macromolecules

P12.07.24

Determination of the contrast mechanism in ultra-small-angle X-ray scattering (USAXS) imaging

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Ultra-Small-Angle X-ray Scattering (USAXS) imaging has been proven useful in studies of metallurgical, biological and polymeric materials. This is a size sensitive imaging technique to directly probe the morphology and three-dimensional arrangements of the small-angle scattering objects, where images acquired at different scattering vectors can reveal different microstructural features within the same sample volume. Until now, the contrast mechanism has not been explained quantitatively. We offer a general treatment of X-ray imaging contrast for USAXS imaging that makes use of phase propagation and dynamic diffraction theory to account quantitatively for the intensity distribution in the detector plane. Simulated results from a model system of micron-sized spherical SiO_2 particles embedded in a polypropylene matrix show good agreement with experimental measurements. Simulations by means of an alternative geometrical ray-tracing method also account for the features in

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the USAXS images, and offer a complementary view of the small-angle X-ray scattering contrast mechanism. The ray-tracing analysis indicates that refraction, in the form of Porod scattering, and, to a much lesser extent, X-ray reflection, fully account for USAXS imaging contrast.

Keywords: small-angle X-ray scattering, synchrotron radiation imaging, image simulation

P12.07.25

Analysis of solution small-angle scattering using the program package ATSAS

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Small-angle scattering (SAS) of X-rays and neutrons is a universal technique serving as a nanometer structure probe for a wide variety of non-crystalline objects (e.g. solutions of biological macromolecules, nanocomposites, alloys, synthetic polymers etc). The program package ATSAS [1] implements advanced methods for the data analysis from isotropic systems, developed for but not limited to, biological mactomolecules in solution The package allows one to perform major analysis steps of the scattering data from data reduction to automated three-dimensional (3D) modelling. With the present ATSAS 2.2 version it is possible:
to compute overall structural parameters and characteristic functions;
to reconstruct ab initio 3D low resolution shapes;
to calculate the scattering profiles from atomic models of macromolecular structures;
to perform rigid body modelling of macromolecular complexes;
to jointly employ X-ray and contrast variation neutron scattering data;
to quantitatively analyze interacting and flexible systems and mixtures.
The use of the ATSAS package is illustrated by the recent examples of its application to study oligomeric state and conformation changes of proteins [2,3], macromolecular complexes and large assemblies [4,5].
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Keywords: SAXS and SANS synchrotron, macromolecular complexes, quaternary structures
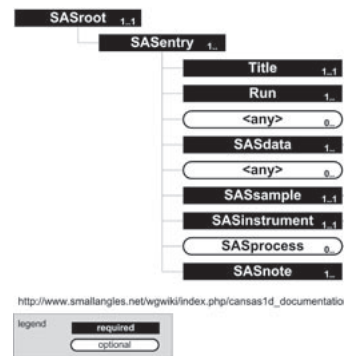
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The canSAS standard for storing reduced one-dimensional small-angle scattering data in XML files

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One of the first aims of the canSAS (Collective Action for Nomadic Small-Angle Scatterers, www.smallangles.net) forum of users and facility staff was to discuss better sharing of SAS data analysis software. CanSAS identified that a significant need within the SAS community is satisfied by standardizing a robust, self-describing, text-based format to communicate reduced one-dimensional small-angle scattering data, I(Q), between users of our facilities. Our goal has been to define such a format with minimal verbosity that leaves the data file instantly human-readable, editable in simple editors, and importable by simple text import filters in programs that need not recognise advanced structure in the file nor require advanced programming interfaces. The file should contain the primary data, I(Q), and also any other descriptive information (metadata) about the sample, measurement, instrument, processing, or analysis steps. The cansas1d/1.0 standard meets the objectives for a 1D standard, incorporating experiment metadata, and parameters and results of processing or analysis steps. Even multiple measurements may be included within a single XML (or SASXML) file.

Keywords: small-angle scattering, standards, data representation

P12.07.27

Software for automated high-throughput biological small-angle X-ray scattering

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Small-Angle X-ray Scattering (SAXS) is a fundamental tool in the study of proteins and macromolecular complexes. SAXS is employed for screening large numbers of samples and for studying these samples under different conditions, including space- and time-resolved analysis. These measurements produce immense amounts of data, especially on modern third-generation synchrotron radiation sources. Automation of data analysis becomes an indispensable prerequisite for adequate evaluation of high-throughput SAXS experiments. We have developed a set of tools to perform major analysis tasks automatically, starting from the raw data processing and finishing with three-dimensional modelling. Automated data analysis starts from raw data reduction including radial averaging of scattering intensities, normalization, radiation damage check, and subtraction of the background. The radius of gyration (Rg) is