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

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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].
References
[1] P.V. Konarev et.al., J. Appl. Cryst. **39** (2006) 277.
[2] E. Mimtsidu et.al., J. Struct. Biol.. **161** (2008) 172.
[3] A. Varga et.al. , BBRC **366** (2008) 994.
[4] X. Zhang et.al. J. Mol. Biol. **362** (2006) 753
[5] H.H. Niemann J. Mol. Biol. (2008) Jan 16 [Epub ahead of print]

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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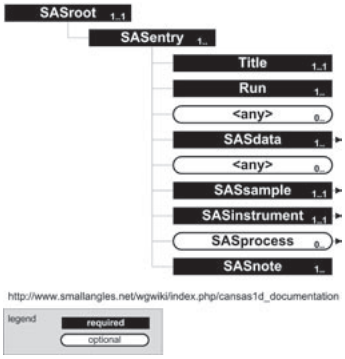
One of the first aims of the canSAS (Collective Action for Nomadic Small-Angle Scatterers, www.smallangles.net) forum of users and facility staff was to discuss better sharing of SAS data analysis software. CanSAS identified that a significant need within the SAS community is satisfied by standardizing 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

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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

computed from the data by Guinier approximation, providing also a quality estimate of the data set. Other overall parameters and the characteristic functions are computed, and, for monodisperse systems, particle shape is reconstructed ab initio. All these steps are assembled in a pipeline running completely automatically without user intervention. The summary of the results including plots and models are stored in XML-based format which gives the possibility to conveniently browse and analyze the results. Decision-making blocks are being developed to select proper analysis actions and to compare concurrent models or suggest experiments reducing the ambiguity of the current model.

Keywords: SAXS, automated data collection, automation

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X-ray reflectivity and grazing-incidence small-angle scattering studies of high-k dielectric films

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Results will be presented from combined X-ray reflectivity and grazing-incidence small-angle X-ray scattering (GISAXS) studies of the nucleation, growth and internal structure of atomic layer deposited (ALD) hafnium oxide (hafnia) films. ALD is an important film growth technique that enables accurate growth of ultrathin layers (1 nm to 3 nm) for high-k gate dielectric materials such as hafnium oxide. The use of a hafnia layer as the gate dielectric on a silicon substrate will play a critical role in extending Moore's Law to the next generation of electronic devices. The X-ray reflectivity yields information on the film thickness, surface roughness and hafnia/Si interfacial region, while GISAXS provides complementary information on the film internal structure and also on the surface roughness and hafnia/Si interface. Furthermore, while reflectivity provides out-of-plane structural information, GISAXS also provides information on the in-plane structure. However, with films this thin, both experiments must be conducted at an X-ray synchrotron source in order to access the high scattering vectors (Q) required. Our studies have explored variations in the hafnia film morphology as a function of different chemical preparations in the ALD process, of film thickness, and also of thermal annealing such as can occur in service thermal transients, etc. By combining the reflectivity and GISAXS data with data from other methods such as Rutherford back-scattering, transmission electron microscopy and electrical measurements, new insights can be gained into the integrity and performance of thin ALD hafnia films used in high-k dielectric gate applications.
[1] M.L. Green, A.J. Allen, X. Li, J. Wang, J. Ilavsky, A. Delabie, R. Puurunen and B. Brijs; Appl. Phys. Lett., 88, 032907 (2006).

Keywords: GISAXS, reflectivity, thin films

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Location of Mn sites in GaMnAs thin films studied by means of X ray diffuse scattering

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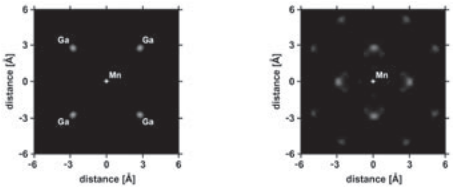
The ferromagnetic properties of $Ga_{1-x}Mn_xAs$ alloys depend on the sites of Mn dopants. The Curie temperature T_C increases with the concentration of the substitutional Mn cations. On the other hand, T_C is strongly decreased by defects, the most important being Mn interstitials. The sites of Mn impurities in $Ga_{1-x}Mn_xAs$ thin films with different concentrations of Mn were studied by means of the X-ray diffuse scattering. An image of the local neighbourhood of Mn atoms in a $Ga_{1-x}Mn_xAs$ (x=0.02) thin film has been obtained by means of X-ray diffuse scattering holography. The positions of the first and second nearest neighbours of the manganese atoms evidence the Mn atoms in substitutional positions (Fig. 1(left)). Moreover, the changes of the local atomic structure of a $Ga_{1-x}Mn_xAs$ (x=0.07) layer during annealing were studied using X-ray diffuse scattering. The difference of pair-distribution functions before and after annealing (Fig. 1(right)) imaged the fraction of atoms that changed by annealing and identified it to be exclusively interstitial atoms. Fig. 1: The local neighbourhood of Mn cations in $Ga_{1-x}Mn_xAs$ thin films with the concentration of Mn (x = 0.02 (left) and (x = 0.07 (right).



Keywords: magnetic semiconductors, X-ray diffuse scattering, holography

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Structure at Fe/NiO(100) and Fe/MgO(100) interfaces by X-ray absorption fine structure

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Interfaces between ferromagnetic (FM) and antiferromagnetic (AFM) films are extensively studied since they exhibit the intriguing exchange bias effect. On the other hand, the interface formation between a FM film and a non-magnetic (NM) material is an interesting system being the constituting elements in tri-layers showing the magnetoresistance effect. NiO is a very promising AFM material for applications, since its Neel temperature is higher than room temperature and MgO is largely used as a spacer between FM films in spin-valve devices. The FM-AFM and FM-NM interfaces constitute the fundamental elements in the design of new magneto-optical devices. Theoretical models of FM-AFM and FM-NM systems often assume an abrupt interface, which must be verified experimentally since the influence of exact interface structure on the magnetic properties of these systems has been demonstrated to be crucial. We have employed polarization dependent X-ray Absorption Fine Structure (XAFS) at the Fe K-edge to investigate the structure at the Fe/NiO(100) and Fe/MgO(100) interfaces. The XAFS measurements demonstrate that the two interfaces present different structures. Indeed, we find [1] that Fe film at the Fe/NiO(100) interface exhibits a complete tetragonal distortion of the unit cell and demonstrate the formation of a buckled FeO layer with expanded Fe-O distances perpendicular to the growth plane. Instead,