Struct. Biol., 2003, **144**, 4.
Keywords: membrane proteins, electron crystallography, methods development

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Atomic Model of Microsomal Glutathione Transferase 1 from Electron Crystallography
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The integral membrane protein microsomal glutathione transferase 1 (MGST1) possesses glutathione and peroxidase activity thus protecting the organism from toxic substances. We have determined the atomic model of MGST1 at 3.5Å resolution by electron crystallography of 2-dimensional crystals from two different two-sided plane groups making it the first membrane enzyme solved to atomic resolution by this technique. The MGST1 homotrimer is constructed by 12 trans-membrane helices forming three all alpha-up-down 4-helix bundles with a fold strikingly similar to the cytochrome c oxidase subunit I suggesting divergent evolution from a common structural ancestor. The MGST1 model reveals inter-subunit interaction and strengthens previous suggestions of global conformational changes upon glutathione (GSH) binding. Furthermore a possible location of the putative hydrophobic binding site is suggested.
Keywords: microsomal glutathione transferase 1, membrane protein structure, electron crystallography

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Structural Features of Cyclodextrin Inclusion Complexes
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Inclusion complexes of α-,β- and γ-cyclodextrins with poly(ethylene glycol)(PEG) and other polymers were prepared using various methods reported so far. The inclusion complexes exhibited the following crystalline features.

1.The inclusion complex of α-cyclodextrin/poly(ethylene gycol) gave a very spotty hexagonal electron diffraction pattern, which gave the hexagonal unit cell. In the case ofβ-cyclodextrin/ poly(propylene glycol), a spotty hexagonal electron diffraction pattern was also observed. The spotty appearance of these electron diffraction pattern is caused by the following host/guest arrangement: The host cyclodextrin columns are arranged in ordered way, even though guest molecules randomly oriented in the caves of dextrin hosts.

2.The inclusion complexe of γ-cyclodextrin with poly(ethylene adipate) gave a "superlattice" comprising 8x8 cyclodextrin units, and additionally its electron diffraction pattern showed the characteristic streaky diffuse scattering due to the attacking fault of the cyclodextrin units.

3.The inclusion complexes contained water molecules in them. The crystal structure was largely disordered, when water molecules were removed by heat treatment. As the original structure was recovered by exposing water vapor, the structural order/disorder transition occurs reversibly.
Keywords: cyclodextrin, superlattice, electron diffraction

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In-situ X-ray Scattering Studies of Nanomaterial Growth Dynamics in Aerosols
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Nanomaterials display unique properties intermediate between those of the molecular and macroscopic regimes. The interest in application of nanomaterials has driven a desire to understand the fundamental mechanisms and processes involved in nanomaterial formation. Generally, nanomaterials are formed under non-equilibrium conditions with deep supersaturation and are commonly formed by extremely rapid growth processes that lead to kinetically dominated structural features. Aerosols offer transient and dramatic changes in temperature, concentration and stoichiometry that can be put to use to produce highly non-equilibrium conditions for nanomaterial formation. Our understanding of nanomaterial formation under these conditions can be studied in situ using synchrotron based techniques. This presentation will highlight some of the most important discoveries made during the past 2 years at ESRF and APS (USA) on flames and environmental aerosols. The work was supported by the Swiss National Science Foundation, the US National Science Foundation and Dupont Corporation.

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Keywords: nanomaterials, nucleation-and-growth, aggregation

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Dynamics of Amphiphilic Systems Probed by Highly Time-resolved SAS Experiments
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Amphiphilic molecules form a large variety of self-aggregating structures that are highly dynamic with time scales ranging from μs to weeks. Often morphological changes can be triggered by mixing with other surfactants, additives, or solubilisates. In our experiments rapid mixing was studied by coupling the stopped-flow technique to high-flux SANS/SAXS instruments which allows to obtain detailed structural information with a time-resolution of 5-50 ms. By this method a large variety of different structural transitions were investigated, e. g. the formation of unilamellar vesicles by admixing oppositely charged surfactant or a cosurfactant. For both cases slow formation of monodisperse unilamellar vesicles is observed that takes place in a way purely governed by diffusion. Both, kinetics and the final structure depend strongly on the electrostatic conditions of the system. In other experiments the disintegration of micelles when mixing with a bad solvent was followed, which passes through a minimum aggregation stage before smaller micellar structures are reformed. This applies also to much larger block copolymer micelles of the PIB-PAA type. Their response to changes of ionic strength and also their complexation with oppositely charged polyelectrolytes was studied. For all cases the details of the transformation can be studied and in particular it is possible to identify intermediate structures, a point which is very important for a systematic control of the dynamics of self-aggregating systems.
Keywords: colloids, amphiphilic molecules, dynamics

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Cytochrome C and αTS Folding Probed by Submillisecond Continuous-Flow SAXS
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Protein folding dynamics is of great interest as being closely related to protein functions and the origin of many diseases. Many proteins collapse within the first hundred of microseconds thus requiring submillisecond-time resolution techniques to observe the effect. At the Advanced Photon Source we have applied a microfluidic continuous-flow mixer and a highly focused X-ray beam at the 18ID beamline in order to study protein folding by small-angle X-ray scattering (SAXS). This made possible to achieve time resolution of about 0.1 millisecond using final protein concentrations as low as 1 mg/ml. Refolding of guanidine-induced denatured state of cytochrome c studied by this technique in submillisecond and millisecond time range demonstrated progressive increase of compactness of the protein molecules indicated by the decrease in radius of gyration from 24 to 15 Å. The SAXS data from the α-subunit of tryptophan synthase demonstrated that the collapse of urea-denatured state of the protein occurred within the first 150 microseconds of dilution experiment. The measured radius of gyration of 33 Å was significantly smaller than that for the denatured state (43 Å). This work was supported by NIH grants RR08630 and GM23303 and NSF grant MCB0327504. Use of the Advanced Photon Source was supported by DOE under Contract No. W-31-109-Eng-38.

Keywords: small-angle scattering, time-resolved studies, protein folding

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Spin Chirality in Non-centrosymmetric MnSi as Probed by Polarised Neutrons

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MnSi is a prototype of a weak itinerant ferromagnet that orders below T=29 K in a left-handed helical spin structure. Because MnSi crystallises in the non-centrosymmetric space group P213 that lacks a center of symmetry the Dzyaloshinski-Moriya interaction (DM) is allowed in this compound. The antisymmetric DM stabilises the spin helix along the [1 1 1] crystallographic axis. Here we will present results of elastic and inelastic neutron scattering experiments performed both below and above the ordering temperature. We will show that because the chemical structure of MnSi is non-centrosymmetric the neutron cross section depends upon the polarisation of the neutron beam. This allows to separate the symmetric from the antisymmetric part of the dynamical susceptibility unambiguously. Consequently it was possible to show that 1) there is only one type of magnetic helix in MnSi in the magnetically ordered state [1], 2) the critical fluctuations in the vicinity of the magnetic phase transition as measured by triple-axis spectroscopy [2] and small-angle scattering [3] have a chiral character. In addition measurements of the dependence of the spin structure under applied magnetic field will be presented.

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Keywords: Dzyaloshinski-Moriya interaction, polarised neutrons, chirality

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Near Field Heterodyne X-ray Speckles

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We report on the observation of stable, low contrast speckles obtained with synchrotron radiation by simply letting static scattered X-Ray radiation fall onto a high resolution camera.

The speckles have circular symmetry, their diameter being typically a few microns. Their size does not change as the sample to sensor distance is varied between few millimeters up to several centimeters. It is argued that the speckles are due to a self-referencing scheme where both the scattered radiation and the heterodyne local oscillator originate from the same rapidly changing, local coherent beam patch.

It is suggested that the X-Ray speckles are of the same type of those obtained with the newly reported optical Near Field Scattering method that has been shown to be equivalent to static light scattering, as the scattered intensity distribution can be retrieved by the statistical analysis of the speckle intensity distribution.

The simple lensless arrangement described above could be used as a new ultra low scattering method operative at extremely small scattering angles where conventional X-Ray scattering methods fail.

Speckle generated X-Ray scattering data are reported for the cellulose acetate filters that exhibit a quasi spinodal structure. A minimum appears at q=0, and an anticorrelation peak at finite wavevectors is also reported. The data are in good qualitative agreement with light scattering data from the same samples.

Keywords: small-angle scattering, Fourier optics, fractals