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Crystals and Beyond. Shelomo I. Ben-Abraham. *Department of Physics, Ben-Gurion University, IL-84105, Beer-Sheba, Israel.*
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I briefly summarize the discussion in the Zeitschrift für Kristallographie on „What is a crystal?" [1]. The best up-to-date answer is that it is a solid whose Fourier spectrum contains a pure point part, in other words, it shows Bragg peaks. That rises the more general question about „What diffracts and how?" Hence, there is growing interest in quasiregular heterostructures [2]. These are layer structures artificially fabricated according to certain algorithms, mainly substitution sequences. Some outstanding examples are Fibonacci, Thue-Morse, Rudin-Shapiro, paperfolding and period doubling chains (finite parts of sequences) [3]. Their spectral properties are of great interest.

[1] *Z. Kristallogr.*, **2007**, 222/6&10. [2] Garcia-Moliner, F. *Microelectronics J.* **2005**, 36, 870. [3] Sloane N.J.A *On-Line Encyclopedia of Integer Sequences,* http://www.research.att.com/~njas/sequences/.

Keywords: crystal definition; quasiregular heterostructures; substitution sequences

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Recent Developments of Multilayer Optics for SAXS in the Laboratory. Nicoleta Galatanu[a], Sergio Rodrigues[a], Vincent Roger[a], Pierre Panine[a]. [a]*Xenocs Sa, 19 rue François Blumet, 38360 Sassenage - France.*
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Since the development of the Guinier camera, small angle X-ray scattering techniques are following the X-ray source progress, with very few innovations on the detectors. Hence, 3rd generation synchrotron source has allowed for significant progress, with milli-second time resolved experiments or by reaching ultra small angle regime, making use of existing detectors. Similar technical trend is also present for laboratory instruments and last year's significant developments in detectors is also giving new potentialities to laboratory SAXS. A key point is the source-to-sample optical coupling to further increase the brilliance in the laboratory to avoid or to prepare experiment in synchrotrons.
Xenocs multilayer optics coupled to microfocused source provide a large increase in photon flux density and enables new science in the laboratory. Indeed, not only liquid crystals or polymers profit from these progresses, but new domains - proteomics, cosmetics, detergents, pharmaceuticals, nanoparticles, catalyzers, food engineering… - are now possible. In the aim to further progress in the q-range and in shortening experimental time, Xenocs developed even higher and more efficient coupling between laboratory sources and samples, with near-to-ideal shape multilayer optics.
In this paper, we will discuss the different properties and expected performances of multilayer optics routinely used in lab SAXS and we will introduce the latest developments with close-to-ideal mirror shape, flux and divergence. It will be shown that microfocused sources and aspheric multilayer optics are ideally suited to provide the most efficient coupling and to get the highest flux with adapted bandpass and divergence to SAXS experiments. Several experimental results will illustrate the usage of such optics either on microfocused sealed tube or rotating anodes.

Keywords: SAXS; multilayer optics; laboratory sources

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SAXS/SANS Structural Analysis of Human Thrombomodulin Domains. Kuo-Long Lou[a], Po-Tsang Huang[a], Guey-Yueh Shi[a], Hua-Lin Wu[a]. [a]*Institute of Biochemistry, Medical College, National Taiwan University. Taipei, Taiwan.*
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Thrombomodulin (TM) is a membrane protein distributed in many different tissues with crucial functions in coagulation and fibrinolysis. Enhancement of blood coagulation function was not supposed to be through blood vessel per se, instead, possibly through pivotal mediations by molecules like thrombomodulin. With such involvement of TM participation, coagulations and immune responses may be bridging in many important aspects. The structures of TM are proposed to be responsible for its functions. The lectin-like domain of TM can be categorized as family containing C-type lectin, which is strongly involved in cell adhesion and inflammations, especially the properties regarding its carbohydrate recognition domain structure. As a consequence, it is absolutely essential to understand the structure of TM, in order to get into more functional details of its regulation in the aforementioned properties. Thrombomodulin (TM) forms a 1:1 complex with thrombin. Whereas thrombin alone cleaves fibrinogen to make the fibrin clot, the thrombin-TM complex cleaves protein C to initiate the anticoagulant pathway. Until present, the so-far available structures, either through NMR or through X-ray analyses, can not shed lights into the decent structural-functional interpretations for TM regulations. Crystallographic investigations of the complex between thrombin and TM-EGF456 did not show any changes in the thrombin active site. Therefore, research has focused recently on how TM may provide a docking site for the protein C substrate with different Ca^{2+} concentration. Previous work, however, showed that when the thrombin active site was occupied by substrate analogues labeled with fluorophores, the fluorophores responded differently to active (TMEGF1-6) versus inactive (TMEGF56) fragments of TM. To investigate this further, we are using SAXS/SANS by carrying out amide $H/^2H$ exchange experiments with thrombin in the presence of active TM-EGF45 and inactive TM-EGF56 fragments. Both on- and off-exchange experiments show changes in the thrombin active site loops, some of which are observed only when the active TM fragment is bound. These results are consistent with

the previously observed fluorescence changes and point to a mechanism by which TM changes the thrombin substrate specificity in favor of protein C cleavage.

Keywords: thrombomodulin; structural analysis; calcium-induced dimerization

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S3-MICROpix: A High-Efficiency SAXS System for the Laboratory. Peter Laggner[a], Philipp Herrnegger[a], Manfred Kriechbaum[a]. [a]*IBN - Institute of Biophysics and Nanosystems Research, Austrian Academy of Sciences, A-8042 Graz, Austria, and Hecus X-Ray Systems GmbH, A-8020, Graz, Austria.* E-mail: Peter.Laggner@oeaw.ac.at

A compact table-top SAXS instrument with high-brilliance X-ray optics in combination with a solid-state pixel detector (Pilatus, Dectris, Villigen, CH)[1)] has been developed on the basis of the Hecus S3-MICRO system (Hecus XRS, Graz)[2)] . The optics consist of a high brilliance microfocus source, a bi-ellipsoidal focussing multilayer element (GeniX, Xenocs, Sassenage, France)[3)], and a tuneable 2-D beam-shaping SAXS-collimator. This provides a monochromatic ($\Delta\lambda/\lambda \geq 10^{-2}$) point-beam of ≤ 0.09 mm^2 cross section with a flux of $\geq 3x10^7$ ph/s, and a divergence of 0,5 x 1 mrad^2 (vert./horiz.). This corresponds to a nominal resolution of ~3000 Å. In practice, it is more relevant to define a quality parameter Θ by the q-value of the pixel, where the ratio of the local background intensity and the integral primary beam intensity is less than 10^{-8}. With S3-MICROpix, $\Theta \leq 5.10^{-3}$Å^{-1}. This high optical quality, which is substantially better than conventional 3-pinhole geometry or ‘parallel beam’ optics, is achieved by focusing the primary beam precisely on the detector plane, by minimising parasitic scattering (windows, slits) and, most importantly, by the ‘zero-noise’ Pilatus-100 detector, overcoming the background problems inherent in conventional CCD detection.

With S3-MICROpix, low-scattering power systems such as protein solutions can be analysed in record times for laboratory SAXS. A test series with lysozyme solution at different exposure times has shown, that exposure times longer than 9 min do not lead to significant improvement of the results in terms of errors in the p(r)-function. The radius of gyration can be determined within less than 3 minutes to an error of ≤ 2%. This sets a new standard for nano-particle sizing.

Other high-brilliance dependent techniques, such as GISAXS, high-pressure experiments (up to 100 MPa), time-resolved 2D-SWAXS experiments (static or flow-through) and automated high-throughput screening are implemented in the compact table-top system (floor space ≤ 4 m^2 including system control station).

The system provides a highly energy-saving alternative to traditional laboratory SAXS-stations since the X-ray source is operated at 50 W, as compared multi-kW power normally used for laboratory instruments.

[1]http://www.dectris.com/sites/pilatus100k.html [2] http://www.hecus.at/pdf/S3-MICROpix.pdf [3] http://www.xenocs.com/range-beam-delivery-systems.htm.