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Ultra-Small-angle X-ray scattering—X-ray photon correlation spectroscopy: A New measurement technique for *in-situ* Studies of equilibrium and nonequilibrium dynamics

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Ultra-small-angle X-ray scattering—X-ray photon correlation spectroscopy (USAXS-XPCS) is a new measurement technique for the study of equilibrium and slow nonequilibrium dynamics in disordered materials. Taking advantage of Bonse-Hart crystal optics, this technique fills a gap between the accessible scattering vector ranges of dynamic light scattering and conventional X-ray photon correlation spectroscopy. It also overcomes the limits of visible light scattering techniques imposed by multiple scattering and is suitable for the study of optically opaque materials containing near-micrometer sized structures.

USAXS-XPCS has been applied to study the equilibrium dynamics of micrometer-sized colloidal dispersions and nonequilibrium dynamics of polymer composites and alloy steels. We anticipate that this technique will be important in the understanding of thermally-induced equilibrium dynamics of soft materials and nonequilibrium behavior of both soft and hard materials, and lead to technical payoffs in a wide range of areas such as the manufacture of advanced ceramic and metallurgical materials and self-repairing biologically critical materials.

[1] F. Zhang, A.J. Andrew, L.E. Levine, J. Ilavsky, G.G. Long, A.R. Sandy, *Journal of Applied Crystallography* **2011**, *44,* 200-212.

Keywords: ultra-small-angle X-ray scattering, X-ray photon correlation spectroscopy, dynamics.

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RDF studies on microstructural changes in coir fibre by the action of enzymes

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This work reports radial distribution functional (RDF) analysis of x-ray intensities diffracted by coir fibres(lingo-cellulose in nature) obtained from kerala,India and that of the same coir fibres treated with enzyme laccase and xylanase(to do away with lignin,hemi-cellulose,pectin and waxy materials) and consequently changes in inter-atomic distances,coupling constants [1] and mean square displacements [2] from the position and breadth of the every peak in RDF pattern were calculated. Although inter-atomic distances do not change significantly, the coupling constant and mean square displacement changes considerably suggesting improvement in mechanical properties of the enzyme treated coir fibres. This was further corroborated by the measurement of tensile strain of treated and untreated fibres.

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COD: an open access tool for searching and retrieving crystallographic Data

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The Crystallography Open Database (COD) is a large collection of CIF files (now ~140000), for inorganic, metal-organic and small organic crystal structures, with the goal of complete coverage in the future. Data are in an SQL database so that structures can be searched by unit-cell parameters, chemical composition or any text (including authors, titles, ...). Data and searching engine are open-access available at http://www.crystallography.net and at mirrors worldwide. The main driving idea behind COD is that the enormous volume of non-copyrightable crystallographic data produced by scientists should be available as freely and easily as possible to anybody without restriction. Nowadays technologies make it possible that an Open Database is maintained by a group of volunteers, while data are directly uploaded by researchers.

Created in 2003, after Michael Berndt's challenge, the initial team lead by Prof. Armel le Bail installed a main COD server at the Univeristé du Maine, Le Mans, France. The server later moved to the Institute of Biotechnology at Vilnius, Lithuania, at the end of 2007, where most of COD development is currently carried out under Dr. Saulius Gražulis supervision. After the last reported description of COD [1], new features were implemented and will be presented here. COD is distributed for phase identification through calculated powder patterns by most XRD manufacturers (Brucker, PANalytical, Rigaku).

Actual COD development involves two main tasks: gathering more data and developing software for uploading, searching and retrieving CIFs. Two major increases in CIF file number came from the AMCSD donation (2003) and from the 2007 decision of the IUCr of providing journal data availability to all databases. At present, the largest data source is automatic direct downloading of CIFs from journal websites performed by COD contributors or automated web crawlers. In addition, the COD website recently incorporated an automatic deposition service, where checking of the syntax and for the presence of essential data in the incoming files is done on-line and the resulting data are made available to the community immediately after deposition or after the subsequent publication if the depositor chooses so. The new COD website enables simultaneous cooperation of several COD editors and has sped up the COD growth considerably.

The next step in software development should be to include a substructure search engine into COD websites, since this is probably the chemically most important way of searching compounds. Performing such searches requires extraction of chemical connectivity from COD CIFs and storage in an appropriate format. Currently SMILES is chosen for this and, for a subset of the database, this information is already available for use in free search software tools. An experimental version of the substructure search engine should be available soon for searches on a fraction of the database.

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