MS32 O1

Fully 3D: Shaping future synchrotron beamline strategies Sandor Brockhauser[a], Marco Di Michiel[b], Raimond B.G. Ravelli[a] [a]*EMBL Grenoble Outstation, 6 rue Jules Horowitz, 38042 Grenoble, France.* [b]ESRF, 6 rue Jules Horowitz, 38043 Grenoble, France.
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Keywords: tomography, absorption correction, macromolecular crystallography

The anomalous scattering properties of innate sulphur for proteins and phosphorus for DNA and RNA can be used to solve the phase problem in macromolecular crystallography (MX) via the single-wavelength anomalous scattering method (SAD). However, this method, used at longer X-ray wavelengths (1.5 - 2.5 Å), is still not a routine tool on third generation synchrotron macromolecular crystallography beamlines. The increased absorption from both sample and air associated with the use of longer X-ray wavelengths forms one of the difficulties to overcome. The absorption can be corrected for through empirical algorithms, provided truly redundant data are available. Unfortunately, weakly diffracting macromolecular crystals suffer from radiation damage, resulting in dose dependent non-isomorphism, which violate the assumption these empirical algorithms are based on. An analytical correction scheme based on an accurate 3D description would overcome the need of redundant data. We show how to obtain the 3D description of vitrified macromolecular crystals, the surrounding solvent and sample holder, and discuss possible benefits and needs to reorient these objects to arbitrary orientations.

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Diffraction mapping of hierarchical systems Gavin Vaughan[a], Jon Wright[a], Carsten Gundlach[a], Lawrence Margulies[a,b], Søren Schmidt [b], Henning F. Poulsen [b], [a]*ESRF, Grenoble, France,* [b]*Risø Nat. Lab., Roskilde, Denmark,* E-mail: vaughan@esrf.fr

Keywords: Materials Science applications of Synchrotron Radiation; Polycrystal Crystallography; Hierarchical Characterization.

A variety of methods (reviewed in [1]) based on high-energy X-Ray diffraction have been developed to characterize crystalline samples on length scales ranging from 100s of nm to mm. These methods have been used to characterize a variety of systems of interest to materials science such as metals and alloys, ceramics, hydrogen-storage materials and components from the microelectronic industry. All of these materials have in common that their performance or macroscopic properties are heavily influenced by sub-micron characteristics such as grain boundaries, crystallite orientations, stoichiometry gradients, etc., and in order to fully understand these systems characterization on several length scales is necessary.
In this talk, we will review briefly the current techniques at our disposal and our ongoing efforts to extend them via both software and hardware developments. The main drive of this research is to be able to treat arbitrary crystalline samples as an ensemble of single crystallites, as the individual properties of those crystallites, as well as their inter-relationships, are ultimately more important to the understanding of the systems in question that simple bulk average properties. A variety of analytical methods, coupled with their experimental realizations, have been implemented on a purpose-built station at the ESRF

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Protein Crystal Processing by Femtosecond Laser and Pulsed Deep-UV Laser Kazufumi Takano[a,b,c], Hiroaki Adachi[a,b,c], Hiroyoshi Matsumura[a,b,c], Satoshi Murakami[a,b,c], Tsuyoshi Inoue[a,b,c], Yusuke Mori[a,b,c], [a]*Osaka University,* [b]*CREST-JST,* [c]*SOSHO Inc., Osaka, Japan.* E-mail: ktakano@mls.eng.osaka-u.ac.jp

Keywords: protein crystal, processing, laser

We have developed novel techniques of protein crystal processing by femtosecond laser [1, 2] and pulsed deep-UV laser [3-5]. The techniques, named as fs-CACO (femtosecond-laser-induced cut and cleave operation) and PULSA (pulsed UV laser soft ablation), are effective for processing and manipulation of protein crystals without significant damage. By fs-CACO, a protein crystal is precisely processed without mechanical contact in its sealed growth vessel. PULSA enables us to process a single crystal both in crystallization drop and in nylon loop and cryoprotectant at a cryogenic temperature [6, 7]. A crystal processed by PULSA can be re-grown larger than its original size, as a single crystal [8]. We also applied these techniques to detaching protein crystals from a fused-silica glass plate [9] or capillary tube [10]. These techniques are powerful tools for handling fragile protein crystals and improving diffraction data quality.

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[10] Kashii *et al.*, *J. Biosci. Bioeng.* 2006, 102, 372.

MS32 O4

Absorption Correction based on a 3D Crystal and Support Model Ricardo Leal[a,b,c], Susana Teixeira[a,b], Vicente Rey-Bakaikoa[b], Edward Mitchell[b], Trevor Forsyth[a,b]. [a]*School of Chemistry and Physics, Keele University, UK.* [b]*European Synchrotron Radiation Facility, Grenoble, France.* [c]*Institut Laue-Langevin, Grenoble, France.* E-mail: ricardo.leal@esrf.fr

Keywords: absorption correction, machine vision, modeling

During the merging and scaling of raw crystal diffraction data several corrections are made (e.g. Lorentz, polarisation and crystal decay). Amongst them there is one which is to be developed in this work: the absorption correction. Due to non-uniform crystal and crystal support

shape the intensities of the same Bragg reflection and its Friedel mate, will be recorded in the detector with different values. This is especially significant at low energies.
There are several methods to calculate the coefficient of transmittance over the crystal and its support. Although the theory of this calculation is very well known, so far there is no efficient method to calculate this factor in macromolecular crystallography for low redundancy data. It is also well known that the best methods to calculate this factor take into consideration the shape of the crystal. However, due to several constraints, especially the often tiny size and highly irregular shape of the crystals, it is often difficult to define a crystal shape.
Taking advantage of the standard resources available at all of the ESRF and ILL MX beamlines and following a strong computer vision and 3D reconstruction approach, this project is developing a method to calculate the abortion correction based on the actual crystal and support shape.

MS32 O5

An Image Processing Approach to Diamond Inspection and Evaluation, Moshe Porat, *Department of Electrical Engineering, Technion, Haifa, Israel.*
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Keywords: diamonds, nondestructive evaluation, machine vision

Diamonds and other gemstones have always been thought to be the symbol of beauty, however, most of these gemstones still contain small natural inclusions and man-made defects. These defects interfere with the passage of light through the crystal and affect its brilliance and appearance, thereby influencing the quality and value of the crystal. Traditionally, diamond impurities are examined by experts with lens and tongs. Obviously, this kind of manual inspection is subjective and sometimes ends with misleading descriptions due to the varying standards. In addition, such expert-based examination or grading is costly and time consuming [1], [2].
In recent decades, new inspection tools, such as ultrasonic and X-ray, have been introduced to the crystal defects detection effort, however, it requires relatively expensive equipment and still cannot meet the demands. On the other hand, recent developments in image processing and computer vision offer an opportunity to use new tools in the gemstone inspection area, especially for diamonds. Understanding the defect type and other key features of a diamond can also be achieved by applying pattern recognition technology [3]. A computer vision inspection system offers a way to recognize the 3Cs (Clarity, Color, Cut-Style) features of diamonds, which are among the diamond's important 4Cs (adding 'Carat' to the above 3Cs). By applying expert evaluation knowledge, systems can readily grade diamonds. Furthermore, since the type, location and size of the defects are particular to each diamond, this inspection approach provides a means to identify a gemstone according to the feature records in a database, so that diamonds may be recognized and traced for future handling.
We focus on defect detection methodology and capturing major features of the diamond, including the structure and defects type. A new recognition approach is proposed to efficiently extract these features, to record their history, and to grade or classify the information in order to identify a gemstone. This approach includes shape analysis, color representation, pattern matching, spectral analysis, image retrieval and image registration. We investigated the use of wavelets and curvature measurement to approximate a diamond shape, and pattern recognition is used to help match the vertex points; Spectral localized descriptors are used to represent the crystal's shape, modified and normalized to cope with potential geometric transformations of the diamond due to various view points. The unique optical features of a crystal are extracted by computer vision operations, and de-noising tools are applied to remove noise. Similar patterns are retrieved by color and shape. Image registration and similarity measurement are also implemented. The system and its performance are presented along with practical results based on actual diamonds. Our conclusion is that the new approach to diamond inspection and recognition could be very helpful in the field of diamonds and similar gemstones evaluation.

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