remotely. Beamline I03 has recently been upgraded with a Pilatus 6M detector running at 25 Hz. This leads to an increase in throughput and allows for new methods like faster grid scans for locating hardly visible samples or to find the best area of a larger sample. We also provide data collection strategies and crystal and diffraction image characterization automatically. Very shortly after the data collection has finished the results from our automatic data processing pipeline are available and we have extended this now to the generation of difference electron density maps if a suitable PDB file is provided.

In order to adapt to the future scientific requirements of the structural biology community we are in the process of installing new experimental end-stations on the Phase 1 beamlines. The first of these has recently been installed on beamline I04 and details will be presented elsewhere.

In addition to the beam delivery by a bimorph KB mirror system providing typical beam sizes of 90 µm x 30 µm over the complete energy range, the new end-station is also equipped with two sets of compound refractive lenses (CRL) providing a beam size of 10 x 4 microns. This presents an additional challenge on the performance of the collimation system components, especially beam diagnostics for beam intensity and position measurements. Some new developments and preliminary results will be discussed. The new end-station also provides the possibility to add a mini kappa goniometer head and preparation work is ongoing for this.

Future capabilities will include category 3 pathogenic sample handling (I03) and an adaptable and improved software user interface. An update on these developments will also be presented.

[1] http://www.diamond.ac.uk [2] http://www.diamond.ac.uk/Home/Beamlines/MX.html

Keywords: diamond light source, macromolecular crystallography, beamlines

MS07.P14

Acta Cryst. (2011) A**67,** C260

Structural evolution of poly(ether-*b*-amide12) elastomers during uniaxial drawing studied using in-situ synchrotron WAXS and SAXS

Soo-Young Park,[a] Tahseen Kamal,[a] and Young-Wook Chang,[b] [a]*Department of Polymer Science and Engineering, Kyungpook National University, Daegu, Korea.* [b]*Dept of Chemical Engineering, Hanyang University, Ansan, (Korea).* E-mail: psy@knu.ac.kr

Poly(ether-b-amide)s have been commercially known as PEBAX. The general structural formula of these block copolymers is HO-[CO-PA-COO-PE-O]-H where PA and PE are polyamide and polyether blocks, respectively. Atochem© uses nylon 12 and poly(tetramethyle neoxide) (PTMO) for PA and PE blocks, respectively, for a PEBAX series with trade names of PXX33 where XX represents the amount of the PA measured by hardness of the block copolymer.[1-2] Structural evolution of PEBAX elastomers during uniaxial drawing was studied using in-situ WAXS and SAXS for elucidating hierarchical morphological development using a synchrotron radiation source with two distinctive block copolymers having different amounts of the soft and hard segments, P6333 and P2533 which represents a soft elastomer and a hard rubber, respectively. The in-situ SAXS and WAXS tracked morphological change of the lamellar, the crystal structure of nylon 12 block, and strain-induced crystallization of the polyether block. High flux of x-rays at a synchrotron made it possible to acquire structural information during sample stretching in real time which was beneficial over the methods used in the past by holding the samples at specific strain.

Several kinds of the nylon 12 crystal such as γ, α, α′, and α″ were observed at the different draw ratios during drawing PEBX film. P2533 has much longer polyether block than P6333. Long polyether block of P2533 could cause not only the strain-induced crystallization but also the fibrillation of the stretched chains. Short polyether block of P6333 prohibited the strain-induced crystallization and transferred the stretching force into the lamellae of the nylon 12 crystal so that the anisotropic crystal lattice deformation was observed only for P6333.

[1] G. Deleens, P. Foy, E. Marechal, *Eur Polym J* **1977**, *13,* 337. [2] G. Deleens, ANTEC **1981**, *419.*

Keywords: PEBAX, synchrotron, elastomer

MS07.P15

Acta Cryst. (2011) A**67,** C260

Facilities for Macromolecular Crystallography at BESSY II – HZB Berlin.

Manfred S. Weiss, Martin Bommer, Ronald Förster, Michael Hellmig, Michael Krug, Karthik Paithankar, Sandra Pühringer, Michael Steffien, Uwe Mueller, *Helmholtz-Zentrum Berlin für Materialien und Energie, Institute F-I2, Macromolecular Crystallography, Albert-Einstein-Str. 15, D-12489 Berlin, (Germany).* E-mail: msweiss@helmholtz-berlin.de

The Macromolecular Crystallography (MX) group at the Helmholtz-Zentrum Berlin (HZB) has been in operation since 2003. Since then, three state-of-the-art synchrotron beam lines (BL14.1-3) for MX have been built up on a 7T-wavelength shifter source [1,2]. Currently, the three beam lines represent the most productive MX-stations in Germany, with more than 500 PDB depositions. BLs14.1 and 14.2 are energy tunable in the range 5.5-15.5 keV, while BL14.3 is a fixed-energy side station (13.8 keV). All three beam lines are equipped with CCD-detectors. Beam lines BL14.1 and BL14.2 are in regular user operation providing about 200 beam days per year and about 600 user shifts to approximately 50 research groups across Europe. BL14.3 has been equipped with a HC1 crystal dehydration device and has been set back to user operation as a screening and test beam line in 2010. BL14.1 has recently been upgraded with an MD2-microdiffractometer including a kappa-geometry option and an automated sample changer. Additional user facilities include office space adjacent to the beam lines, a sample preparation laboratory, a biology laboratory (safety level 1) and high-end computing resources. On the poster, a summary on the experimental possibilities of the beam lines and the provided ancillary equipment for the user community will be given.

[1] U. Heinemann, K. Büssow, U. Mueller, P. Umbach, *Acc. Chem. Res.* **2003**, *36*, 157-163. [2] U. Mueller *et al.*, in preparation.

Keywords: synchrotron, beam line, macromolecular crystallography

MS07.P16

Acta Cryst. (2011) A**67,** C260-C261

Colliding Beam Anomalous Measurements for S and P Phasing

James M. Holton,[a,b] Kenneth A. Frankel,[b] Alastair A. MacDowell,[b] John C. H. Spence,[c] [a]*Biochemistry and Biophysics, University of California, San Francisco (USA).* [b]*Lawrence Berkeley National Laboratory,1 Cyclotron Rd., Berkeley, CA (USA).* [c]*Department of Physics, Arizona State University, Tempe, Arizona 85287, (USA).* E-mail: JMHolton@lbl.gov

Phasing macromolecular crystals (MX) with native elements such as sulfur and phosphorous has many advantages over heavy atom substitution methods, but it has always been hampered by systematic errors. At their K edges, sulfur (2.5 keV) and phosphorous (2.1 keV) exhibit comparable anomalous signal strength to that of selenium (f" ≈ 4 e^-), but conventional MX data collection is impractical at these wavelengths because the attenuation depth in protein crystals is only ~20 μm. Not only are the diffracted beams weak, but the uncertainty in the attenuation factor itself is a systematic error that is generally greater in magnitude than the anomalous difference to be measured. Using smaller crystals reduces the attenuation factor as well as the error it introduces, but at the expense of increasing another systematic error: radiation damage. In general, crystals small enough to have small absorption errors do not survive long enough for accurate anomalous differences to be measured. To date, successful sulfur phasing experiments have used relatively large crystals of sulfur-rich proteins and photon energies of about 7 keV. However, the new technique of femtosecond nanocrystallography has demonstrated significant reduction of radiation damage effects and good data quality at 2 keV from crystals much smaller than the attenuation depth. Unfortunately, each crystal may only be shot once, and it is geometrically impossible to simultaneously place a given h,k,l index and its Friedel mate (-h,-k,-l) onto the same Ewald sphere, so two opposing Ewald spheres must be generated. This is accomplished by illuminating the crystal with two X-ray beams, coming from opposite directions for a Colliding Beam Anomalous Measurement (CBAM). In this geometry, the diffracted rays of each Friedel pair emerge from the crystal in opposite directions with identical partialities and very similar attenuation factors. This makes it possible to directly measure the relative Bijvoet difference (ΔF/F) without any need to integrate the full spot intensity and circumvents the "partiality problem" of single-beam femtosecond nanocrystallography. At the sulfur K edge, 2.5 Å data may be collected, provided the detector surfaces are arranged to cover most exit angles, including backscattered rays. The simultaneous recording of patterns from two Ewald spheres does increase the likelihood of overlaps, but this is compensated by the "still" nature of the patterns. The design of a CBAM instrument for use at the Linac Coherent Light Source is currently underway.

Keywords: sulfur phasing, XFEL, femtosecond, nanocrystal

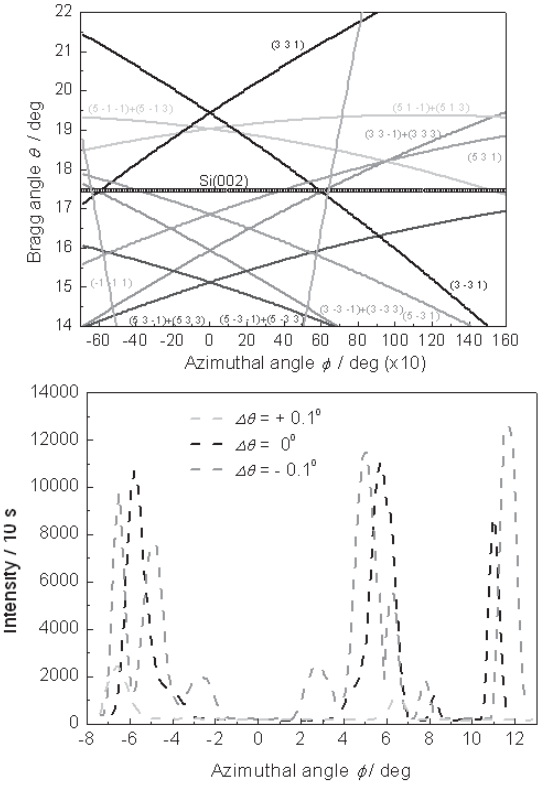
MS07.P17

Acta Cryst. (2011) A**67,** C261

Multiple Bragg Reflections in Cylindrically Bent Perfect Crystals

Pavol Mikula,[a] Miroslav Vrana,[a] Jan Saroun,[a] Vyacheslav Em,[b] B.S. Seong,[b] [a]*Nuclear Physics Institute ASCR, v.v.i., Rez (Czech Republic).* [b]*Neutron Science Division, KAERI 1045 Daedok daero, Yuseong-gu, Daejeon, 305-353 (Republic of Korea).* E-mail: mikula@ujf.cas.cz

Multiple Bragg reflections (MBR) realized in one bent-perfect crystal (BPC) slab by sets of different lattice planes behave differently in comparison with the case of perfect nondeformed or mosaic crystal. Individual sets of lattice planes are mutually in dispersive diffraction geometry and the kinematical approach can be applied on this MBR process. Then, MBR process can be considered as one or several parallel double Bragg reflection events. By using neutron diffraction and the method of azimutal rotation of the Si crystal around the scattering vector related to the forbidden primary reflection (002) at the wavelength 0.1625 nm, several strong multiple reflections were investigated with a possible exploitation in high resolution diffractometry. The intensities of the monochromatic beam obtained on the basis of MBR effect depend on the thicknes of the crystal and its curvature as well as on the orientation of the individual participating planes with respect to the crystal deformation vector.



Keywords: neutron diffraction, multiple reflections, bent perfect rystals

MS08.P01

Acta Cryst. (2011) A**67,** C261-C262

Modulation of microtubule protofilament interactions by modified taxanes

José Manuel Andreu,[a] Ruth Matesanz,[a] Javier Rodríguez-Salarichs,[a,b] Benet Pera,[a] Angeles Canales,[a] Jesús Jiménez-Barbero,[a] Wim Bras,[c] Aurora Nogales,[d] Wei-Shuo Fang,[e] José Fernando Díaz,[a] [a]*Chemical and Physical Biology, Centro de Investigaciones Biológicas, CSIC. Ramiro de Maeztu 9, 28040 Madrid, (Spain).* [b]*Centro de Estudios Avanzados de Cuba. Carretera San Antonio km 1 1/2 , Valle Grande, La Lisa, Ciudad Habana, CP. 17100, Cuba.* [c]*Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO), DUBBLE CRG/ESRF BP 220 F38043 Grenoble Cedex, France.* [d]*Instituto de Estructura de la Materia, CSIC, Serrano 121, 28006 Madrid, (Spain).* [e]*Institute of Materia Medica, Chinese Academy of Medical Sciences, 1 Xian Nong Tan Street, Beijing 100050, China.* E-mail: j.m.andreu@cib.csic.es

The antitumor compounds paclitaxel (taxol) and docetaxel modify the association between αβ-tubulin molecules promoting their assembly into microtubules. These drug-induced microtubules have different numbers of protofilaments [1]. The modification of the microtubule structure, through a non-yet characterized mechanism, is probably related to the changes in the tubulin-tubulin interactions responsible of the stabilizing activity. The effects of taxanes modified in positions C2, C7, C10 and C13 [2] on microtubule structure have been characterized using Small Angle X-ray Scattering. Modifications in positions C7, C10 and C2 result in changes of interprotofilament angles and thus in alterations of the microtubule structure, while modifications in position C13 do not induce any changes.

The observed effects have been explained using NMR-based