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

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Multiple Bragg Reflections in Cylindrically Bent Perfect Crystals

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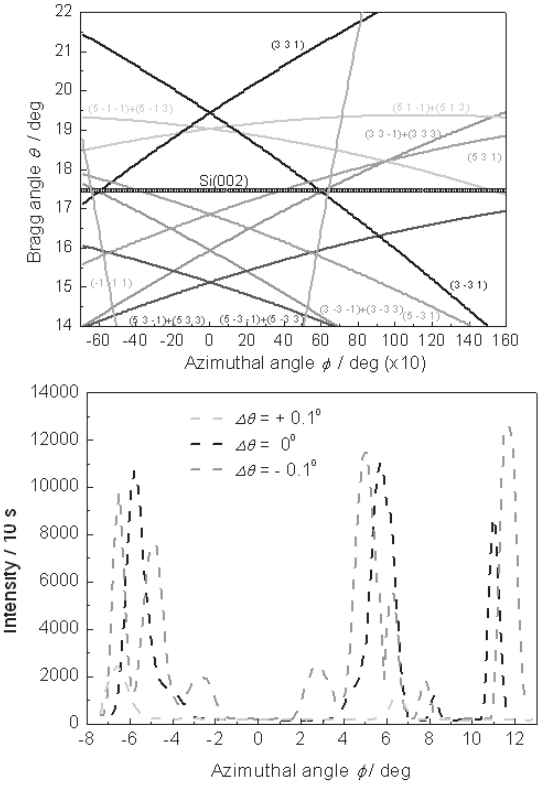
Multiple Bragg reflections (MBR) realized in one bent-perfect crystal (BPC) slab by sets of different lattice planes behave differently in comparison with the case of perfect nondeformed or mosaic crystal. Individual sets of lattice planes are mutually in dispersive diffraction geometry and the kinematical 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

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Modulation of microtubule protofilament interactions by modified taxanes

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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