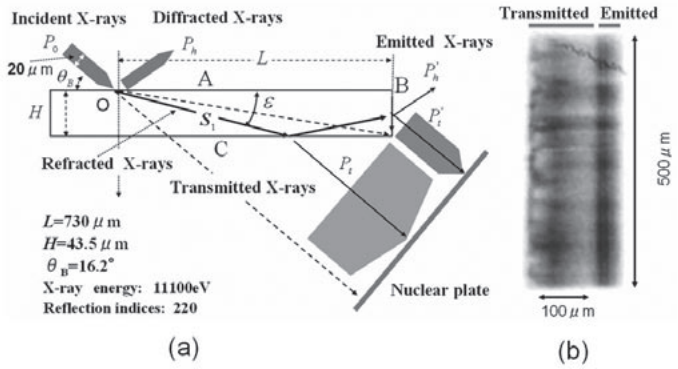
observed as the transmitted beams. The ratio of the dispersion angle $\delta\varepsilon$ of the refracted beams with respect to $\delta\theta$ ($\delta\varepsilon/\delta\theta$) becomes approximately 10^5. This means that the diffraction in this case works as a lens, which is quite useful for development of X-ray microscope, high resolution monochromator and X-ray interferometer.



Keywords: Bragg case, dynamical diffraction theory, X-ray microscope

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New mechanism of anomalous transmission, absorption and their additional unusually curious feature

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The recursion formulas of the photon paths in the Borrmann triangle (BT), which satisfies a modified Bragg law [1, 2] could be derived from the binomial distribution (BD) of the *n*-multiple X-ray reflections by regarding the permutation of the stochastic variables of the diffracted and transmitted photons. Sub-BT of the diffraction shows perfectly flawless symmetry but that of the transmission shows inevitable asymmetry. Novel understanding of both the high intense and very weak photon flows in BD, which are known as anomalous transmission and absorption, respectively are revealed from BD approximated to the standard normal distribution of $N(0, 1)$. Incident photons into the vertex "O" of BT propagate through the bypasses parallel to only the complementary half of the integral whole median with the high probabilities from the binomial theorem and emanate them from a very narrow slit of $O'O''$ on the base of the high intense photon flow BT of $\Delta OO'O''$, which could be defined by the standard deviation of $N(0, 1)$. The parallel paths to the whole median also pass as the very weak photon flows from the high exponent of $d^{-n}t^{-0}$ in *n*-degree homogeneous multinomials of *d* and *t* through the triangle $\Delta OO'O''$. It could be undetectable owing to the negligible small of $1/{}_nC_{\sim n/2}$ compared with the high intense photon flows. It is for this reason that X-ray photons never emerge from the crystal at a position, which is directly opposite the entrance point on a straight line on the diffraction plane. Therefore, an additional unusually curious feature could be clearly understood from the above.

[1] T. Nakajima:J. Low Temp. Phys. **138** 1039-1075 (2005).
[2] to be presented in this conference

Keywords: dynamical diffraction, transmission, absorption

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The influence of mosaic distribution upon the extinction factors in real crystals

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The evaluation of a series of wide ranging tables of secondary extinction factors Y for the spherical mosaic crystal, requires a detailed comparison of the numerical solutions of Darwin transfer equations for cylindrical crystals with different sorts of mosaic distributions [1]. Three probability functions t (n) were used: t (infinity) is close to Gaussian (G), t (1) is Lorentzian (L) and t (2) closely resembles the Lorentzian but the "tail" is shorter. From the figure one can see that when the ratio of absorption cross section to scattering cross section is small and the sample radius is large, the areas under the rocking curves, i.e. integrated reflection power ratio (IRPR), differ appreciably. The corresponding secondary extinction factors Y, which are proportional to IRPR, for G, L and t (2) are 0.0402, 0.1016 and 0.0781, respectively. The Y, for L distribution is 30% higher than that of the t (2). Thus it seems that the most reasonable mosaic distribution for real crystals would be G or t (2) but not L. This result may serve as a guideline for the evaluation of the appropriate extinction table.

[1] Hua-Chen Hu. Acta Cryst. A59, P. 297-310. (2003).

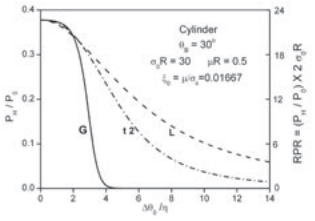

Fig. 1 Rocking curves from three different mosaic distributions for cylindrical crystals.
μ : absorption cross-section.
σ : scattering cross-section.
σ_0: σ at $\Delta\theta_0$.

Keywords: diffraction physics, mosaicity, extinction

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Absorption coefficient of X-rays in crystals in presence of temperature gradient

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The behavior of factor of linear absorption of X-rays in monocrystals on Laue geometry is experimentally investigated and shown, that the presence of a temperature gradient and ultrasonic vibration leads to essential reduction of absorption of X-rays. In the present work the theoretical analysis of the given process in plane wave approximation, in the presence of a temperature gradient is carried out. The theoretical analysis shows that (with beam penetration in a crystal) the presence of the curvature leads to the increase of amplitude diffracted and weakly absorbed field and simultaneously to the reduction of amplitudes of diffracted and strongly absorbed field and as well as amplitude of both passing fields. With magnification of curvature of reflecting atomic planes, transferred energy in diffracted weakly absorbed field is increases and the total energy is transferring via this field at certain value of curvature. As a consequence the crystal absorption coefficient sufficiently decreases. The further magnification of curvature, leads to reduction of energy transferred

via diffracted weakly absorbed field (the absorption coefficient is again increased). For the explanation of the above mentioned processes the total intensity of transversed and diffracted bunches in the Darwin's table region are analyzed at different curvatures of reflecting atomic planes. It is obtained, that with reduction of the radius of curvature the total intensity at Bragg exact angle, and over all region of Darwin's table is increased, i.e. the absorption coefficient decreases. Theoretical calculations have been carried out for a quartz single crystal for several families of reflecting atomic planes. However the above mentioned effect was most brightly observed for reflecting (10-11) planes.

Keywords: X-ray attenuation coefficient, dynamical X-ray diffraction theory, crystal lattice distortion

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Portable thermal platform for optimising protein crystallisation

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The major parameters affecting protein crystallisation have been reported and some, such as pH, ionic strength, and purity of chemicals have been successfully controlled during the entire crystallisation experiment. However temperature is a parameter that still remains elusive. Several strategies have been developed to control temperature during the crystallisation process. These include the use of temperature-controlled rooms, thermostated cabinets, temperature-controlled instrumentation prototypes and modified PCR thermocyclers. To date, the current systems have the disadvantage of failing to control and record temperature changes once the sample is removed from them. These temperature fluctuations occur several times during the crystallisation experiment e.g. while inspecting the crystals under the microscope, or when selecting and mounting the crystals for X-ray diffraction. This work reviews the current state of the art in temperature control for protein crystallisation and presents an effort to actively control and record the temperature during the entire crystallisation experiment. The system presented is an electronically controlled portable temperature control platform for screening and optimising protein crystallisation. The system is designed in the form of a double height 96 well pitch microplate where five different temperatures can be screened and monitored simultaneously. The performance of the system and crystallisation results using a number of proteins will be presented.

Keywords: temperature, optimisation, crystallisation

P16.01.02

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In situ proteolysis for protein crystallization and structure determination

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Obtaining well-diffracting crystals remains the main bottle-neck in protein crystallography. Analysis of large-scale structural genomics projects (http://targetdb.pdb.org) reports 10~15% success rate in obtaining the structure-quality crystals from a given set of purified proteins. Thus vast majority of proteins submitted to conventional crystallization trials either do not crystallize or form poor quality crystals, which can not be used for structure determination. We present here a general rescue technique, named in situ proteolysis, allowing 15~20% increase in successful crystallization. Our method is based on observation that trace amounts of protease present in the protein sample may lead to formation of hydrolyzed protein fragment prompt to crystallization. To test if addition of protease can be used as general crystallization technique we selected 55 bacterial protein samples from the pool of Midwest Centre for Structural Genomics targets. Of the 55 proteins, 20 had previously failed to crystallize and 35 had formed crystals that were unsuitable for structure determination. Addition of chymotrypsin protease to each protein sample prior crystallization trials (in 1:100 ratio) resulted in obtaining structure quality crystals for eight proteins. The Trypsin and subtilisin protease addition to the remaining protein samples allowed obtaining three additional protein structures. The analysis of eleven solved structures demonstrated that in every case the polypeptide chain forming the crystal lattice was partially degraded by protease. The relative simplicity and significant increase in successful crystallization makes this method a prominent rescue technique in protein crystallization.

Keywords: *in situ* proteolysis, protein crystallization, chymotrypsin

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In situ proteolysis for protein crystallization and structure determination

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Analysis of large-scale studies (http://targetdb.pdb.org) shows that, of all proteins that enter crystallization trials, two-thirds will not crystallize, and half of those that do crystallize can not be optimized to form suitable crystals for structure determination, for a final success rate of ~15% from purified protein to structure. Given the resources that are invested to generate a purified, concentrated protein and to perform extensive crystallization trials, this level of attrition is of considerable concern. The general applicability of in situ proteolysis to form protein crystals suitable for structure determination was tested by adding chymotrypsin or trypsin to crystal trials of a test set of 70 bacterial and human proteins that had proven recalcitrant to our best efforts at crystallization or structure determination. 13 structures were determined from this test set, which more than doubled the success rate of structure determination from purified protein. Application of the method to more bacterial and human proteins has already yielded 10 additional structures, 5 from prokaryotes and 5 from human.

Keywords: *in situ* proteolysis, protein crystallization, chymotrypsin