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Eval15: accurate data integration by profile prediction

X. Xian, A.M.M. Schreurs, L.M.J. Kroon-Batenburg

Crystal and Structural Chemistry, Utrecht University, Padualaan 8, 3584 CH Utrecht, the Netherlands

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We have developed a new reflection data integration method, Eval15, that uses profile prediction. It has the potential of integrating complicated reflection data, such as arise from anisotropic crystal shape, anisotropic mosaicity, a1,a2 splitting, overlap due to twin lattices. At the same time Eval15 has the advantage of accurate integration of weak intensities as a result of profile fitting. It is a follow-up of Eval14 [1], a reflection box-integration method that uses calculated boundaries based on a few physical crystal and instrument parameters. Eval14 is well established for the integration of small molecule data and is especially useful in problematic cases. Weak reflections, however, are not integrated as accurately as it is done by profile fitting methods. This is cumbersome for protein data where the structure determination relies on the accuracy of weak data. The principle of general impact used by Eval14 to predict the reflection boundaries are now used to predict the complete profile of the reflection, that can then be used as a standard profile in a profile fitting algorithm. Every reflection has its own predicted profile that is based on the same physical parameters as in Eval14.In the present contribution we show the first data integrated by Eval15. For small molecules Eval15 has a comparable quality as Eval14 and for proteins it produces data comparable to the profile learning methods Denzo and Mosflm.

[1] A.J.M.Duisenberg, L.M.J. Kroon-Batenburg and A.M.M. Schreurs (2003). *An intensity evaluation method: EVAL-14. J. Appl. Cryst. 36, 220-229.*

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Possibilities of Controlling an X-ray Beam with a Crystal Subjected To Ultrasonic Vibrations

A.E. Blagov

Shubnikov Institute of Crystallography, Russian Academy of Sciences, Moscow, Russia, E-mail: aopt@ns.crys.ras.ru

X-ray diffraction in crystals subjected to ultrasonic deformation is an actively developing field in the solid state physics. In many works researchers aimed to obtain information on the structure of elastic vibrations using X-ray diffraction.

In this work the possibilities of controlling the parameters (amplitude, space position, internal structure and wavelength) of an X-ray beam by means of ultrasound are discussed.

Three main kinds of interaction for different relations between the ultrasonic wavelength λ and the crystal size of surface area, illuminated by an X-ray beam D are considered. Realization of X-ray amplitude modulation could be simply made in all three cases.

The special attention is paid to earlier scantily investigated area of long-wave ultrasound λ>>D. In this area, ultrasound can create the tunable deformations similar to configurations, which used in X-Ray optics.

The way of creation variable in time and uniform or gradient in space deformations is described. This method is based on Laue diffraction in a crystal, subjected to standing ultrasonic longitudinal vibrations.

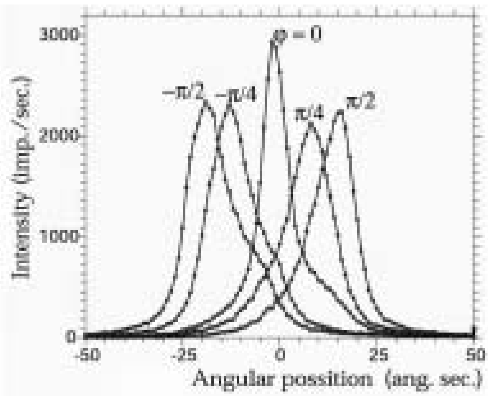
Changeable in time and uniform in space deformations could be used for deflection of X-ray beam or tuning X-ray wavelength.

Changeable in time and gradient in space deformations could be used for focusing, collimation or defocusing X-ray beam.

Experimental setup for longitudinal wave ultrasonic X-ray interaction, including a stroboscopic system for time resolution experiments, is described.

Rocking curves (RC), measured at various resonator vibration phases and various deformation distributions are presented.

RCs, measured under conditions, where an X-ray beam passed through the uniform deformation crystal area, shows the possibility to vary an angular position of diffracted X-ray beam (fig 1).



The forms of RCs, measured where an X-ray beam passed through the crystal area with gradient deformation, shows the possibility to control the spatial characteristics of diffracted X-ray beam. In this case the RC half-width was widened tenfold.

Some special experimental results of momentary static deformation compensation by dynamical ultrasonic deformation are presented. (In this case the RC half-width was compressed ~tenfold).

A theoretical model for X-ray diffraction by a crystal with slowly varying ultrasonic deformation was developed by V. Kohn. The results of calculation, based on this model are compared with experimental results. The profiles of ultrasonic deformation within the X-Ray beam, calculated with using this theoretical model are demonstrated.

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