s4.m1.p3 The factors of polarization transformation of X-ray scattering in Laue-case for dislocation crystals.
N.M.Olekhnovich and A.V.Pushkarev, *Institute of Physics of Solids and Semiconductors, National Academy of Sciences of Belarus, P.Brouki 17, 220072 Minsk, Belarus, e-mail: pushk@ifttp.bas-net.by*
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X-ray diffraction polarization phenomena caused by the dynamical character of scattering are the basis for the development of X-ray polarimetry, diffraction-polarization analysis of real crystals, polarization interferometry and other fields. In the Laue-case of X-ray diffraction with coherent σ and π components of electrical vector of incident wave the effect of birefringence is known. The effects of birefringence and depolarization were found for the real crystals [1]. These appear to depend on the dislocation density and the angle of deviation of the crystal from the Bragg position. It was found, that the parameter of diffraction birefringence κ ($\kappa=\delta/t$, δ is phase difference between the σ and π components, t is the length of optical way of the beam in the crystal) for crystals with the large dislocation density, as distinct from perfect crystal, decreases smoothly with deviating the crystal from the Bragg position and its absolute value is many times smaller than that for the perfect crystal. Such a behavior of this parameter for the dislocation crystals is connected with the factors determined the diffraction process in such crystals. These factors can be estimated while investigating the character of diffraction polarization transformation for reflections of various order. The aim of this paper is to investigate the characteristics of birefringence and depolarization of the transmitted X-ray beam in the Laue case (reflections 002, 022, 004) in the LiF crystals with dislocation density 10^4-10^5 mm^{-2}. It has been found that the effects of diffraction birefringence and depolarization are observed for all the investigated reflections. The parameter κ is shown to depend on the diffraction order and dislocation density. The comparison of the value κ for dislocation crystal with its value for the perfect one (κ_p) is given. The dependence $ln(\kappa/\kappa_p)$ as function of the square of reciprocal lattice vector H^2 has been found. The analysis of this dependence has shown that the value of κ for dislocation crystal is determined by the static Debye-Waller factor and the factor of the effective thickness of the crystal (Δ). The factor Δ is related to the half-width of scattering curve. It decreases as the dislocation density and diffraction order increase. The static Debye-Waller factor for the investigated crystals has been determined from the polarization data. The decrease of depolarization degree of the transmitted beam with the increasing dislocation density and diffraction order correlates with the varying of the factor of the crystal effective thickness.

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s4.m1.p4 Femto-second pulsed Radiation: Comparison between X-ray and electron scattering.
P. Daniels [1], J. Hajdu [2], R. Neutze [2], D. van der Spoel [2], E. Weckert [1], A. Zuev [1]. *(1) Institut für Kristallographie, Fakultät für Physik, Universität Karlsruhe (TH), Kaiserstr. 12, D-76128 Karlsruhe, Germany (2) Department of Biochemistry, Uppsala University, Box 576, S-751 23 Uppsala, Sweden.*
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Planned free electron laser facilities are expected to produce X-ray as well as electron pulses in the femto-second domain which may allow the extraction of structural information from photons or electrons coherently scattered by only one single biological macro molecule. Presently, the behaviour of molecules subject to short X-ray pulses is modelled using the molecular dynamics software package GROMACS[1]. For estimating the amount of energy deposited in a molecule during a radiation pulse and the coherently scattered radiation, accurate cross section data are required.

Three main effects can be distinguished in the case of X-rays: Photo absorption[2], Compton scattering[3], and Rayleigh scattering[4]. The respective cross sections were derived from the references cited. Only the latter effect carries structural information, while the first two deposit energy in the molecule and contribute to the background. For the inelastic scattering of electrons (in the range 100keV-1MeV) no suitable cross section data are available. Only a semi-empirical formula for stopping powers (dE/dx) could be found[5]. Data for elastic electron scattering amplitudes an the other hand could easily be obtained[6].

The beam diameters in both cases were taken to be 1µm and the pulses contained 10^{13} photons and $6 \cdot 10^9$ electrons, respectively. For the comparison of integrated coherently scattered radiations a resolution of up to 1Å was used. As an example we chose lysozyme.

With these data and assumptions the deposited energies and numbers of scattered photons and electrons were calculated. For X-rays the typical value of 12 keV leads to 1.6 fJ deposited by Compton scattering and to 43.1 fJ deposited by photo absorption while 4.8 photons would be scattered elastically. Electrons with an energy of 100keV leave about 24.1 fJ behind in the molecule while the coherent scattering yields 557 electrons. The comparison shows that the energy deposited is in both cases under the given circumstances comparable while the yield of detectable coherently scattered radiation differs by two orders of magnitude favoring the use of electrons if such pulses at the required energy level will ever become feasible.

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