

11.6-05 "FORBIDDEN" REFLECTIONS DUE TO ANISOTROPIC POLARIZABILITY OF CRYSTALS. By V.E.Dmitrienko, All-Union Research Institute of Physical-Technical and Radiotechnical Measurements, Moscow, U.S.S.R.

The effect of the anisotropy of X-ray polarizability on the conditions limiting possible reflections is discussed. If crystallographically equivalent atoms have differently oriented anisotropy of polarizability, they have different scattering power and the "forbidden" reflections may be excited (D.H.Templeton and L.K.Templeton (1980), *Acta Cryst.*, **A36**, 237). In the present work some unusual properties of these reflections are treated in detail.

The symmetry properties both of the tensor of X-ray susceptibility $\hat{\chi}(\vec{r})$ and of its Fourier coefficients $\hat{\chi}_H$ are determined. It is shown that these symmetry properties may result in nonvanishing of even those $\hat{\chi}_H$ which are identically zero if the known reasons (such as nonspherical electron distributions and anharmonicity and anisotropy of thermal vibrations (B.Dawson (1967) *Proc. Roy. Soc.*, **A298**, 255; V.A.Belyakov (1971) *Fiz. Tverd. Tela*, **13**, 3320)) are taken into account. Such reflections have been observed in white tin (B.Borie (1978) *Phys. Stat. Sol.*, **47**, K39; D.W.Field, *ibid.*, **K43**).

From the symmetry properties of $\hat{\chi}_H$ it is also shown that the intensity and polarization properties of the 001 ($l=2n+1$) forbidden reflections in TiO_2 (rutile) are smoothly dependent on the angle of rotation about the [001] axis. Another example is given by screw-axis forbidden reflections with elliptic or even circular polarization of reflected beam. These unusual properties of considered reflections are useful for their experimental observation.

11.6-06 DIFFRACTION BIREFRINGENCE AND DICHOISM OF X-RAYS IN CRYSTALS. By V.E.Dmitrienko and V.A.Belyakov, All-Union Research Institute of Physical-Technical and Radiotechnical Measurements, Moscow, U.S.S.R.

The diffraction corrections to refractive index, birefringence and dichroism of X-rays in crystals are theoretically examined in assumption that X-ray beam is out of Bragg condition. It is shown that in this case the diffraction correction from each reflection $\hat{\chi}_H$ is rather small (approximately $\hat{\chi}_H \hat{\chi}_H^{-1} \sim 10^{-11} - 10^{-12}$; $\hat{\chi}_H$ is the Fourier coefficient in the expansion of susceptibility), but the sum over all reflections has measurable value. For example, the diffraction correction $\Delta n = 2 \cdot 10^{-9}$ for LiF and $\Delta n = 2 \cdot 10^{-8}$ for Ni; both values were calculated for the wavelength $\lambda = 1.54 \text{ \AA}$ and for X-ray beam propagating along [001] direction. Although these corrections are very small, they should be taken into account in the precise interferometric determination of atomic scattering factors. Note that: 1) Δn is strongly dependent on the wavelength and the propagation direction; 2) Δn is weakly dependent on crystal perfection and its value may be determined from the dynamical diffraction theory or from the relevant theory for mosaic crystals (V.E.Dmitrienko and V.A.Belyakov (1980) *Acta Cryst.*, **A36**, 1044).

If the angular deviation of propagation direction from the Bragg one $\Delta\theta$ for some reflection H is not too large ($\Delta\theta \ll 1$ but $|\Delta\theta| \gg |\hat{\chi}_H|$), the diffraction corrections to the refraction index are mostly due to this reflection. For σ and π polarized waves these corrections are

given by the following relations: $\Delta n_\sigma = \hat{\chi}_H \hat{\chi}_H^{-1} / (\Delta\theta \sin 2\theta_B)$ and $\Delta n_\pi = \Delta n_\sigma \cos^2 2\theta_B$. It should be emphasized that Δn_σ and Δn_π rather slowly (as $\Delta\theta^{-2}$) decrease with $\Delta\theta$ increasing (for comparison, the intensity of reflected beam decreases as $\Delta\theta^2$). The birefringence and dichroism are given by the real and imaginary parts of $\Delta n_\sigma - \Delta n_\pi$ respectively (usually, $|\text{Re}(\Delta n_\sigma - \Delta n_\pi)| \gg |\text{Im}(\Delta n_\sigma - \Delta n_\pi)|$). Note that diffraction dichroism is connected with the "tails" of anomalous absorption because it is proportional to $\text{Im}(\hat{\chi}_H \hat{\chi}_H^{-1})$.

The parameters of the X-ray quarter-wave plate are calculated for different crystals. It is shown that due to absorption only light element crystals may be used for transformations of X-ray polarization. For the III reflection in diamond the angle $\Delta\theta$, optimal for the polarization transformation, varies from 1° to 10° if λ changes from 3 \AA to 0.5 \AA respectively (V.E.Dmitrienko and V.A.Belyakov (1980) *Fiz'ma v Zh. Tekhnich. Fiziki*, **6**, 1440). In this case the intensity of Bragg-reflected wave is negligible (less than 1%) and absorption is not large ($\mu L = 1$; μ is the absorption coefficient and L is the plate thickness).

The discussed here off-Bragg quarter-wave plate may be useful for the transformation of the linear polarization of synchrotron radiation into circular one. Note also that measurements of Δn_σ and Δn_π outside the Bragg reflection bands may, in principle, be used for extinction free determination of structure amplitudes.

11.6-07 OPTICAL ACTIVITY AND THE FARADAY EFFECT AT X-RAY FREQUENCIES. By M. Hart and A.R.D. Rodrigues*, Wheatstone Laboratory, King's College, Strand, London WC2R 2LS, UK.

During the last three years considerable progress has been made in developing methods and making measurements of X-ray optical polarization effects (M. Hart, *Phil. Mag.*, (1978) **B38**, 41, M. Hart and A. R. D. Rodrigues, *Phil. Mag.*, (1979) **B40**, 149).

Initial experiments investigated linear and circular birefringence and dichroism. In the experiments which we present here, we have re-examined optical activity in quartz and made systematic measurements on Nickel sulphate hexahydrate paying careful attention to the systematic elimination of Bragg reflections. Earlier results which purported to show the effects of optical activity in silicon (G. G. Cohen and M. Kuriyama, *Phys. Rev. Lett.* (1978) **40**, 957), are re-interpreted in terms of well known Bragg reflection phenomena.

We will report measurements of the Faraday effect in nickel, cobalt, iron and beryllium which give upper bounds of 5°cm^{-1} , 50°cm^{-1} , 50°cm^{-1} and $0.08^\circ \text{cm}^{-1}$ respectively using $\text{CuK}\alpha_1$ radiation. These values are typically 10 times smaller than the values expected on classical theories. Further work is planned at synchrotron radiation sources where the X-ray wavelength can be chosen to be very close to the appropriate absorption edges and where much higher intensities can be achieved with both linearly and circularly polarized X-ray beams.

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