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Polarization ratio for X-ray diffraction by perfect unicrystals with finite thickness.

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Abstract

The polarization ratio is expressed by $|\cos 2\theta|^n$, where 2θ is the angle between the incident and the diffracted rays. For a perfect uniblock single crystal, n is usually taken to be equal to 1. For an ideally imperfect crystal, n is taken to be 2. Any other value of n is attributed to the extent of mosaicity. Numerical computation of the polarization ratio for a perfect nonabsorbing single crystal of infinite lateral extension but finite thickness shows that n, instead of having the constant value of 1, may have any value between 1 and 2, depending on the thickness of the slab, the structure factor of the reflecting plane, the volume of the unit cell and the angle of scattering. The numerical computations are based on Zachariasen's theory of diffraction of X-rays by perfect crystals [Zachariasen (1945). *Theory of X-ray Diffraction by Crystals*. New York: John Wiley].

1. Introduction

The electric vector **E** representing X-rays diffracted by a crystal in any permitted direction $\langle hkl\rangle$ can be resolved into two mutually perpendicular components $\mathbf{E}_\sigma$ and $\mathbf{E}_\pi$. $\mathbf{E}_\sigma$ is the component normal to the plane containing the incident ray and the Bragg reflected ray. $\mathbf{E}_\pi$ is the component lying in this plane. When the incident beam is unpolarized, the intensity of the diffracted beam is

$$I = \langle E_\sigma^2\rangle + \langle E_\pi^2\rangle,$$

the averaging being carried out over all orientations of the electric vector representing the incident X-radiation. The ratio $R = \langle E_\pi^2\rangle/\langle E_\sigma^2\rangle$ is known as the polarization ratio. Darwin (1922) showed that $R = |\cos 2\theta|^n$, where 2θ is the angle of deviation of the diffracted beam with respect to the incident beam and $n = 1$ for an ideally perfect crystal while $n = 2$ for an ideally imperfect mosaic crystal. Ramaseshan & Ramachandran (1953, 1954), Chandrasekharan (1955, 1959) and Chandrasekhar, Ramaseshan & Singh (1969) observed that, in many crystals, n had values lying between 1 and 2 and attributed this to the extent of perfection or of mosaicity in the crystals studied. Similar studies were made by Mitra & Samantaray (1972, 1975) and Calvert, Killean & Mathiesen (1957), in which it was implicitly accepted that the deviation of n from 1 was due to the extent of mosaicity in the crystals studied. Theoretical calculations by Olekhnovich (1969, 1975; Olekhnovich, Rubtsov & Schmidt, 1978) were also based on this hypothesis. Stephan & Loschau (1976) observed that $n = 0\cdot5$ gives better agreement with some experimental data and attempted to explain this theoretically on the basis of a mosaic block model. However, no study seems to have been carried out so far to calculate the value of n for a uniblock perfect crystal with finite thickness or even a semi-infinitely extended perfect crystal. For such cases, except probably for a very thin crystal with thickness approaching zero, n has been taken automatically to be 1, while for thin films n has been taken to be 2. It is important to find out if n for such cases can be different from 1. This is because the prevalent practice would automatically characterize the crystal as mosaic if n has a value other than 1. It is surprising that this problem has escaped the attention of workers in this field since the theoretical formulae needed for such studies have been available for a long time.

2. The Zachariasen theory and its consequences

Zachariasen (1945) derived an expression for X-rays reflected from a perfect crystal with infinite lateral dimensions but finite thickness. A workable formula has been given by Hirsch & Ramachandran (1950) for very thick crystals and by Wilkins (1978) for finite thicknesses. Wilkins (1978) considers a nonabsorbing crystal as an unphysical one but agrees that even a very small absorption factor renders the case physical. As is evident from numerical results of Hirsch & Ramachandran (1950), James (1963) and Wilkins (1978), rocking curves calculated for crystals of zero and negligibly small absorption are almost identical. Thus, considerations for crystals with zero absorption are expected to be qualitatively valid for real crystals. Now, for perfect crystals, *i.e.* uniblock crystals with infinite lateral extension but finite thickness, Zachariasen (1945) derived an elegant expression for the reflecting power for nonabsorbing crystals, *viz*

$$\rho = \frac{|P\chi|\tanh A}{\sqrt{b}\,\sin 2\theta}, \tag{1}$$

where

$$A = \frac{e^2|F|\,Pt\lambda}{mc^2\,v\sqrt{\gamma_0\,\gamma_B}};\quad \chi = \frac{e^2|F|\lambda^2}{\pi mc^2};$$

$$\gamma_0 = \mathbf{n}\,.\,\mathbf{u}_0;\quad \gamma_B = \mathbf{n}\,.\,\mathbf{u}_B.$$

$\mathbf{u}_0$ and $\mathbf{u}_B$ are unit vectors in the direction of incident and Bragg reflected beams respectively. n is a unit vector normal to the diffracting crystalline slab, $P_\pi = \cos 2\theta$ for the π component and $P_\sigma = 1$ for the σ component of the electric vector representing the Bragg reflected ray. $b = \sqrt{\gamma_0/\gamma_B}$, t is the thickness of the slab, V is the volume of the unit cell; F is the crystal structure factor for the reflecting plames; e, m, c are the electronic charge, the electronic mass and the velocity of light in vacuum respectively; λ is the wavelength of the X-rays diffracted. Thus, the polarization ratio is given by

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$$R = \frac{P_\pi}{P_\sigma} = \frac{P \tanh Px}{\tanh x} = |\cos 2\theta|^n, \tag{2}$$

where

$$x = \frac{e^2 \lambda |F| t}{mc^2 v \sqrt{\gamma_0 \gamma_B}}.$$

It is obvious that for $t \to \infty$, $R = |\cos 2\theta|$ and for $t \to 0$, $R = |\cos 2\theta|^2$ as is expected from the Darwin (1922) theory.

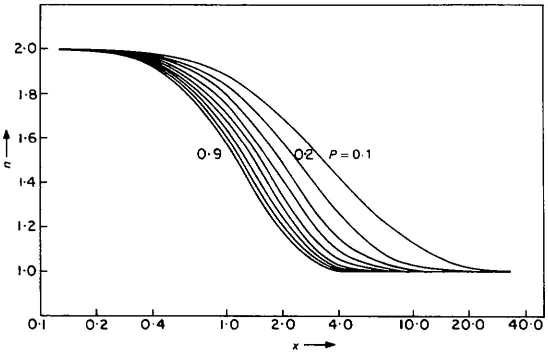

Fig. 1. Variation of n with respect to x for various values of P, as calculated from (2).

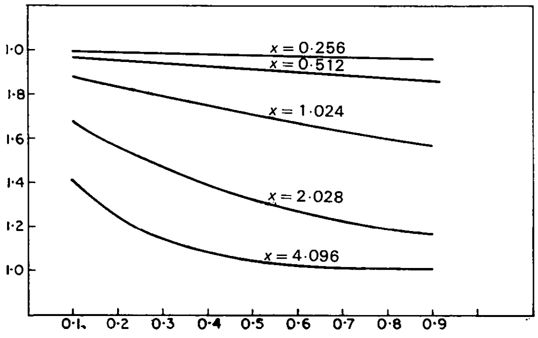

Fig. 2. Variation of n with respect to P for various values of x as calculated from (2).

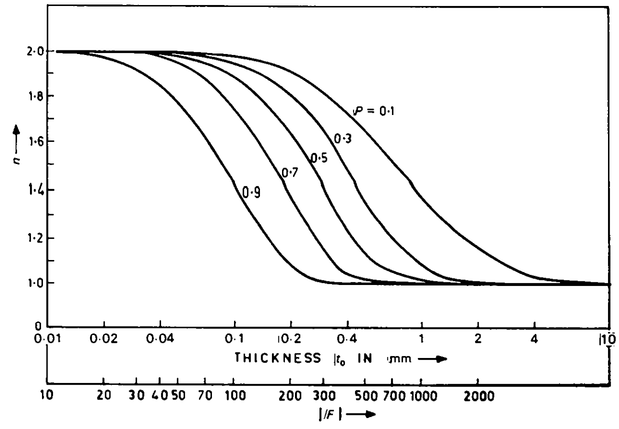

Fig. 3. Variation of n with respect to (i) thickness t (for $F = 100$), and (ii) structure factor F (for $t = 0{\cdot}1$ mm), for various values of P. The values are calculated from (2).

It is also obvious that for different values of t (intermediate between the two extreme cases mentioned above), $|F|$, V and $|\cos 2\theta|$, n will take values other than the expected value of 1. Numerical computations based on (2) have been carried out to determine n in terms of (1) x; (2) P for different values of x, (3) t for different values of P. $|F| = 100$, $\lambda = 1{\cdot}54$ Å and $V = 10^3 \times 10^{-21}$ mm^3 and (4) $|F|$ for different values of P, $t = 0{\cdot}1$ mm, $V = 10^3 \times 10^{-21}$ mm^3, $\lambda = 1{\cdot}54$ Å. They all show values of n lying between 1 and 2 for various conditions for a perfect uniblock crystal with infinite lateral extension but finite thickness. The variations of these factors, calculated from (2), are shown in Figs. 1, 2 and 3.

3. Discussion and conclusions

The present work is not claimed to be an original contribution to the dynamical theory of diffraction or to the theory of diffraction of X-rays by perfect crystals. Equation (2), which is the basis of the present investigation, follows automatically from (1) which is due to Zachariasen (1945). However, the consequences of this equation do not appear to have been appreciated previously. The general conclusion arrived at from this work is that whenever n is found to have a value different from 1 (1·2, 1·6, *etc.*) one should not automatically conclude that the crystal is mosaic or imperfect and proceed to interpret this value of n in terms of extent of mosaicity, dislocation, *etc.* The crystal in this case may very well be a perfect one. Other tests should be applied to find the state of perfection of this crystal.

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