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The X-ray Diffraction of a Bicrystal with a Narrow Plate-Shaped Nondiffracting Zone

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Abstract

The problem of X-ray diffraction by a bicrystalline system containing a narrow nondiffracting zone with an arbitrary smooth profile is theoretically considered. Numerical calculations of the topographic interference pattern intensity distribution *versus* a spatial coordinate are carried out for the case of a nondiffracting zone with parabolic profile.

1. Introduction

X-ray spherical-wave diffraction on a bicrystalline system (BS) with a plane narrow air gap between the crystals was considered by Authier, Milne & Sauvage (1968) and Tanemura & Lang (1973). X-ray diffraction investigations of Si crystals implanted with ions of high energy have been carried out by Bonse & Hart (1969), Bonse, Hart & Schwuttke (1969) and te Kaat & Schwuttke (1972). In these three studies, the existence of a very damaged disc-shaped amorphous zone produced by the implanted ions was revealed. Bezirganyan & Haroutyunyan (1987) and Haroutyunyan & Bezirganyan (1987, 1989) have solved the problem of X-ray diffraction by a bicrystal system with a narrow wedge-shaped air gap. In the air gap as well as in the amorphous region, Bragg diffraction does not occur, therefore these macrodefects are usually called the nondiffracting zone (NZ).

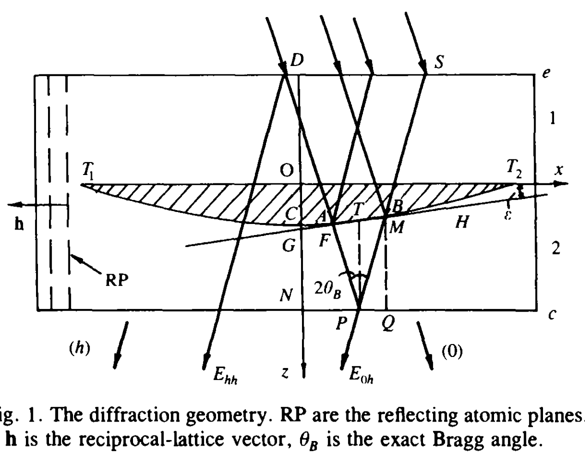

Fig. 1. The diffraction geometry. RP are the reflecting atomic planes, **h** is the reciprocal-lattice vector, θ_B is the exact Bragg angle.

In the above-mentioned studies, the Laue set-up is considered and interference phenomena in the direction of Bragg reflection are studied. In all these cases, a BS is considered as an interferometric BS in which the interference pattern with intensity distribution

$$I_h(x) = |E_{0h}(x) + E_{hh}(x)|^2 \qquad (1)$$

appears. In (1), E_{0h} and E_{hh} are the waves diffracted in the first crystal (or layer) in the directions of transmission (0) and Bragg reflection (h), whereas in the second crystal (layer) of BS both waves are diffracted in the h direction (see Fig. 1; x is the coordinate along the bicrystal exit surface).

However, up to now, the problem of X-ray diffraction by a crystal containing extended NZs with a variable width (in the plane of scattering) has received little attention and has not been strictly considered. In the present paper, this problem is considered for a NZ with an arbitrary smooth profile and for a plate-shaped zone with a parabolic profile.

2. Intensity distribution in the case of a BS containing a NZ with a plate-shaped profile

The problem is considered by us for the Laue set-up under the following assumptions: the incident X-ray wave is plane and monochromatic; the crystal under consideration is a parallel-sided plate and contains a NZ with variable thickness in the plane of scattering; the upper boundary of the NZ is parallel to the entrance surface (e) of the crystal and the bottom boundary has an arbitrary smooth profile given by $z = f(x)$ within the limits $-L < x < L$ (see Fig. 1; the dashed region represents the NZ, xyz is a rectangular coordinate system, $2L = T_1T_2$ is the length of the NZ); the crystal has a perfect structure outside the NZ; X-ray scattering is dynamical under conditions of anomalous Borrmann transmission of X-ray waves in both parts of the bicrystal (owing to the presence of the NZ, a crystal can be considered as a BS; see §1); in the first (upper)

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layer of the BS, Bragg diffraction occurs in compliance with the symmetric reflection scheme.

Besides, suppose fulfilment of the condition

$$|\varepsilon(x)| = |\arctan f'(x)| \simeq |f'(x)| < 10^\circ \simeq 0.2\,\text{rad}, \quad (2)$$

where $f'(x)$ is the derivative with respect to x, $\varepsilon(x)$ is the value of the tilt angle with respect to x of GH tangent at an arbitrary point x in the region $-L < x < L$. For example, in Fig. 1, observation point P at the exit surface of the BS has the coordinate $x = x_0$ and T is the point of contact of the corresponding tangent with NZ interface ($TP \parallel z$ axis). Owing to condition (2), both layers of the BS are simultaneously in position for Bragg reflection, *i.e.* it provides a considerable overlap of the diffraction angular ranges of both layers (Bezirganyan & Haroutyunyan, 1987).

Then let us confine ourselves to the consideration of the case when

$$FM_x \simeq 2\tan\theta_B BQ \ll 2L, \quad (3)$$

where

$$BQ = t_2(x) \simeq -f'(x)x + t_2, \quad (4)$$

$t_2 = CN$ (see Fig. 1), FM_x is the x projection of the section FM of tangent GH, $t_2(x)$ is the thickness of the second (bottom) layer of the BS depending on the x coordinate. From Fig. 1, it can be seen that the section FM is restricted by the column $ATBPA$ whose sides AP and BP coincide with the directions of 0 and h, respectively. The values BQ (the height) and $\angle APB = 2\theta_B$ characterize the dimensions of the column $ATBPA$. Takagi (1969) has shown that the wave field at any observation point P is defined by lattice distortions within the column DSP. In the present case, the curvature of the part ATB of the interface is considered as a 'distortion' within the column DSP. From (2) and (3) and with the assumption that the bottom interface of the NZ has a smooth shape, the curved part ATB of the interface can be approximated by the section FM. Thus, (3) gives us an opportunity to approximate a solution of the present problem, for example, at point $P(x = x_0)$ by the analytical solution of the problem of X-ray diffraction on the BS containing a wedge-shaped gap with the corresponding value of the angle $\varepsilon_0 = \varepsilon(x_0)$. The latter solution has been obtained by us previously (Bezirganyan & Haroutyunyan, 1987). In this approximation, $\varepsilon(x) \simeq$ constant within any column along the NZ, therefore the present approach in a certain sense is analogous to the 'column' approximation, which is widely used in electron diffraction (Hirsch, Howie, Pashley, Nicholson & Whelan, 1965).

Provided that conditions (2) and (3) are fulfiled, replacing in equations (10*a*), (11*b*), (19) and (23) of our previous work (Bezirganyan & Haroutyunyan, 1987) the value ε by $f'(x)$ [see (2)] and assuming that $t_2(x)$ is given by (4), one finds for X-rays that the intensity distribution in the interference pattern formed in the direction of reflection h in accordance with (1) is:

$$\begin{aligned} I_h(x) &= |E_{0h}(x) + E_{hh}(x)|^2 \\ &= (1/16)E^2|\beta_1|^2 b^{-1}|\chi_h/\chi_{\bar h}| \exp\{-(\mu \sec\theta_B + \sin\theta_B m_i) \\ &\quad \times [t_1 + t_2(x)]\}[|A_{0h}|^2 \exp(a) + |A_{hh}|^2 \exp(-a) \\ &\quad + 2|A_{0h}||A_{hh}| \cos\varphi], \end{aligned} \quad (5)$$

where

$$A_{0h} = (-s + m)/mm_1, \quad A_{hh} = (-s_2 + m_2)/mm_2, \quad (6)$$

$$\begin{aligned} \varphi = {} & [-\sin\theta_B(b+1)s + g\sin\theta_B f'(x)]t_2(x) \\ & + 2\sin\theta_B s(t_2 + t_3), \end{aligned} \quad (7)$$

$$m = (s^2 + \beta^2)^{1/2}, \quad m_1 = (s_1^2 + \beta_1^2)^{1/2}, \quad m_2 = (s_2^2 + \beta_2^2)^{1/2}, \quad (8)$$

$$s = K(\theta - \theta_B), \quad s_1 = s - 0.5K\chi_0 \sec^2\theta_B f'(x), \quad s_2 = -s_1, \quad (9)$$

$$\beta = K(\chi_h \chi_{\bar h})^{1/2}/\text{cosec}\, 2\theta_B, \quad \beta_1 = \beta b^{1/2}, \quad \beta_2 = \beta b^{-1/2}, \quad (10)$$

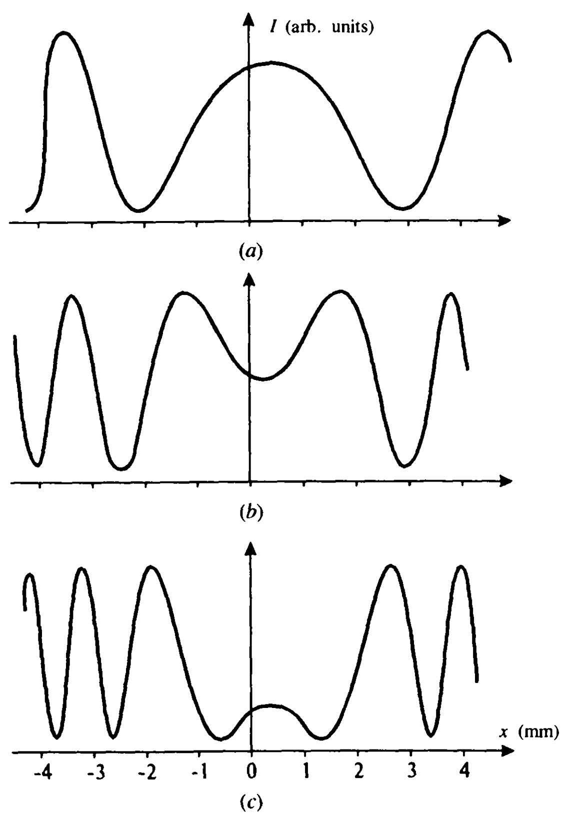

Fig. 2. The plots of the intensity distribution I_h *versus* the coordinate x for t_3 = (*a*) 100 μm, (*b*) 150 μm, (*c*) 200 μm.

$$a \equiv \mu t_2(x) f'(x) \sec\theta_B \tan\theta_B,$$

$$b \equiv \cos[\theta_B - f'(x)]/\cos[\theta_B + f'(x)], \quad (11)$$

$$g \equiv s^2(2\tan\theta_B - 1)/[s^2 + (\beta^2)_r]^{1/2}, \quad (12)$$

$$\mu = K\chi_{0i}, \quad m_i = (\beta^2)_i/2[s^2 + (\beta^2)_r]^{1/2}, \quad (13)$$

E, K, θ and s are the amplitude, the wave number, the angle of incidence and the incidence parameter of the incident wave, respectively; A_{0h} and A_{hh} are the amplitude factors of the waves E_{0h} and E_{hh}, respectively; χ_n is the nth-order ($n = 0, h, \bar{h}$) Fourier coefficient of the polarizability, χ_{0i} is the imaginary part of χ_0, $(\beta^2)_r$ and $(\beta^2)_i$ are the real and imaginary parts of β^2, respectively; $t_1 = OD$ is the thickness of the first layer, $t_3 = OC$, μ is the normal linear absorption coefficient of X-rays. In (10), the values corresponding to the σ-polarization state (polarization factor $c = 1$) of X-rays are given since we consider the case of Borrmann anomalous transmission of radiation.

For a parabolic profile of the NZ (Fig. 1) given by the function $f(x) = (-t_3/L^2)x^2 + t_3$ ($|x| < L$), Si crystal, Mo $K\alpha$ radiation, 220 reflection, $t_1 = t_2 = 3\,\text{mm}$, $2L = 1\,\text{cm}$, $\Delta\theta = \theta - \theta_B = -0.3''$ and, for three values of t_3 (100, 150, 200 μm), the plots of the intensity distribution given by (5) to (13) are represented in Fig. 2. It is obvious that this distribution is very sensitive to change in the NZ shape.

Therefore, from the practical standpoint, it would be interesting to find a solution of the reciprocal problem: reconstruction of the profile of a NZ by its X-ray topographic image recorded on a photographic plate in compliance with the diffraction scheme represented in Fig. 2. The approach developed in the present paper should be useful and effective in consideration of the problems of X-ray diffraction by a single crystal containing an incoherent precipitate, a pore or a crack.

References

Authier, A., Milne, A. D. & Sauvage, M. (1968). *Phys. Status Solidi*, **26**, 469–484.

Bezirganyan, P. H. & Haroutyunyan, V. S. (1987). *Phys. Status Solidi A*, **99**, 37–46.

Bonse, U. & Hart, M. (1969). *Phys. Status Solidi*, **33**, 351–359.

Bonse, U., Hart, M. & Schwuttke, G. H. (1969). *Phys. Status Solidi*, **33**, 361–374.

Haroutyunyan, V. S. & Bezirganyan, P. H. (1987). *Phys. Status Solidi A*, **99**, 329–338.

Haroutyunyan, V. S. & Bezirganyan, P. H. (1989). *Phys. Status Solidi A*, **111**, 41–45.

Hirsch, P. B., Howie, A., Pashley, D. W., Nicholson, R. B. & Whelan, M. J. (1965). *Electron Microscopy of Thin Crystals*. Russian transl. ch. 11, p. 255. London: Butterworths.

Kaat, E. H. te & Schwuttke, G. H. (1972). *Adv. X-ray Anal.* **15**, 504–515.

Takagi, S. (1969). *J. Phys. Soc. Jpn*, **26**, 1239–1253.

Tanemura, S. & Lang, A. R. (1973). *Z. Naturforsch. Teil A*, **28**, 668–676.