

Fig. 2. Difference Fourier section at $z=0.25$ for Pu_3Si_3 . Contours as in Fig. 1.

thus, in the overlapping region, too much electron density was removed.

All calculations were performed with an IBM 7090 or 7094 with programs written by the authors. We wish to thank Mr. V. O. Struebing for preparing the specimen.

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Anomalous Transmission of X-rays in an Elastically Deformed Non-Isotropic Crystal

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A point source of X-rays placed before a slice of dislocation-free germanium produces on a photographic plate behind the slice a picture that is characteristic of the anomalous transmission of the X-rays. The change in this picture due to bending of the germanium slice is explained theoretically in this paper. The characteristic features of the change are related with the fact that germanium is an elastically non-isotropic material.

Introduction

The aim of this paper is to account for certain phenomena connected with anomalous transmission of X-rays through elastically deformed perfect crystals that have been observed by van Bommel (1964) in this laboratory. In his experiments a thin slice of a dislocation-free germanium crystal was irradiated with X-rays from a point source located near the surface of the crystal. A photographic plate some distance away from the opposite surface then clearly indicates the directions in which anomalous propagation of X-ray energy is possible through the crystal. In particular, if the [111] axis of the crystal is perpendicular to the surface, a picture with sixfold symmetry is obtained, which reveals anomalous transmission of X-rays along (220) planes of the germanium lattice. Van Bommel observed that bending of the crystal

results in a characteristic change of the picture on the photographic plate as a result of increased absorption of the X-rays. For instance, bending can destroy the sixfold symmetry of the picture and can produce apparent threefold symmetry. It will be shown in this paper that these experimental results can be understood from the general theory developed in a previous paper (Penning & Polder, 1961) and that they are intimately connected with the cubic anisotropy of the tensor of the elastic compliance of germanium.

Resumé of the general theory

In our previous paper it was emphasized that anomalous transmission of X-rays is connected with the fact that electromagnetic energy cannot propagate as a plane wave in an infinite medium with a dielectric

constant varying periodically in space. Generally speaking, a mode of propagation will be a superposition of plane waves, one of which will predominate for an arbitrary value of its wave vector \mathbf{K} . If this wave vector \mathbf{K} is such that it very nearly satisfies the condition for Bragg reflexion at one particular lattice plane (hkl), two plane-wave components will predominate in the mode. The second plane-wave component will have the wave vector $\mathbf{K}' = \mathbf{K} - \mathbf{K}_{hkl}$, where \mathbf{K}_{hkl} is 2π times the reciprocal-lattice vector characterizing the lattice plane (hkl). If we write $\mathbf{K}_{hkl} = 2\mathbf{b}$, the Bragg condition is satisfied if $\mathbf{K} \cdot \mathbf{b} - \mathbf{b}^2 = 0$. In that case the ratio ξ of the amplitude of the plane-wave component \mathbf{K}' over that of component \mathbf{K} can be either 1 or -1 . The latter sign corresponds to a mode of propagation in which the nodes of the electric field \mathbf{E} of the X-ray coincide with the reflecting planes (hkl), at least if the polarization of \mathbf{E} is chosen to be parallel to these planes. Such a mode suffers the minimum possible absorption and produces the phenomenon of anomalous transmission. It can propagate with little attenuation along the plane (hkl) and escape at the end of the crystal by splitting into two plane waves with wave vectors \mathbf{K} and \mathbf{K}' .

If the Bragg condition is not exactly satisfied the ratio ξ is given by:

$$4(\mathbf{K} \cdot \mathbf{b} - \mathbf{b} \cdot \mathbf{b}) = V_1(\xi^2 - 1)/\xi \equiv 4A \quad (1)$$

where $V_1 = (\omega/c)^2$ times the Fourier component \mathbf{K}_{hkl} of the dielectric constant of the material; it is a negative quantity of the order 10^{13} cm^{-2} . c is the velocity of light in vacuum, ω the angular frequency of the X-ray.

The modes with $\xi \neq -1$, *i.e.* $A \neq 0$, suffer considerably more absorption than that with $\xi = -1$, and the more so the greater the deviation of A from zero. Intense anomalous transmission therefore only occurs for X-rays in a mode with $A \simeq 0$.

In our previous paper we have shown that when an X-ray beam in a given mode propagates inside a bent crystal, the mode parameter ξ or A will not be constant, but will change in a predictable way if the strain, or rather the displacement, in the crystal is a known function of x , y and z . Equation (22) of that paper states that

$$dA = -adl(c^2/\omega)[(\mathbf{K} - 2\mathbf{b}) \cdot \nabla_{\mathbf{r}}](\mathbf{K} \cdot \nabla_{\mathbf{r}})(\mathbf{v} \cdot \mathbf{b}') \quad (2)$$

where dl is a line element in the direction of the group velocity of the mode, a^{-1} the absolute value of the group velocity, \mathbf{b}' the value of \mathbf{b} before deformation, and \mathbf{v} the displacement vector due to deformation. The value of dA/dl must be calculated with the aid of the local values of a , \mathbf{K} , \mathbf{b} and \mathbf{v} on the path of the X-ray beam.

A non-vanishing value for dA/dl will make it impossible for a beam to traverse the entire crystal with minimum possible absorption, since only for

that part of the path for which $A = 0$ is the minimum absorption situation obtained. Therefore, only those beams for which the right-hand side of (2) equals zero in the deformed crystal will not suffer a decrease in (anomalously transmitted) intensity on bending. The quantity

$$[(\mathbf{K} - 2\mathbf{b}) \cdot \nabla_{\mathbf{r}}](\mathbf{K} \cdot \nabla_{\mathbf{r}})(\mathbf{v} \cdot \mathbf{b}'),$$

which is a measure of the intensity decrease on bending, can be written in a different way. Since \mathbf{K} is near to Bragg reflexion anyhow and since, for use in equation (2), \mathbf{K} and \mathbf{b} can be considered as constants, we write

$$\mathbf{K} = \mathbf{d}' + \mathbf{b}', \quad \mathbf{K} - 2\mathbf{b}' = \mathbf{d}' - \mathbf{b}' \quad (3)$$

where \mathbf{d}' is the projection of \mathbf{K} on a plane parallel to the lattice planes (hkl). Incidentally, the direction

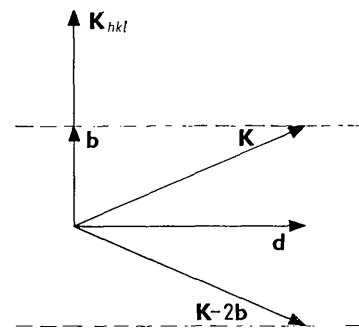


Fig. 1. Definition of vectors \mathbf{b} and \mathbf{d} .

of \mathbf{d}' is also the direction of propagation of a beam with $A = 0$. For a beam with $A \neq 0$ it is still the direction of the projection of the path of the beam on a plane parallel to the reflecting planes. Then (2) can be written as

$$(\omega/ac^2)dA/dl = [(\mathbf{b}' \cdot \nabla_{\mathbf{r}})(\mathbf{b}' \cdot \nabla_{\mathbf{r}}) - (\mathbf{d}' \cdot \nabla_{\mathbf{r}})(\mathbf{d}' \cdot \nabla_{\mathbf{r}})](\mathbf{v} \cdot \mathbf{b}'). \quad (4)$$

This paper will contain the evaluation of (4) for a thin slice of germanium, cut from a single crystal in an arbitrary direction, elastically bent in an arbitrary direction, in which an X-ray beam propagates with a vector \mathbf{d}' of arbitrary direction in a (220) plane. In particular we shall be interested in the case where a [111] direction is normal to the surface of the slice and in the propagation direction \mathbf{d}' for which (4) equals zero.

The elastic deformation

In this section we shall not try to solve the general problem of the elastic bending of a thin slice of solid material characterized by an anisotropic tensor of elastic compliance. The solution strongly depends on

the boundary conditions, *e.g.* on the precise way in which the bending moment is applied. For the evaluation of (4) one needs only the displacement vector \mathbf{v} as a quadratic function of the coordinates x, y, z . For this we need the tensors of the strain and stress as a linear function of x, y, z .

Take as the origin of the x, y, z -system a point Q somewhere in the slice, fixed half way between its front and back surfaces. Bending will cause a stress tensor P , which, to the extent that it is linear in the applied moment, will be written as a power series in x, y, z :

$$P = P^{(0)} + p^{(x)}x + p^{(y)}y + p^{(z)}z + \dots \quad (5)$$

Similarly the resulting strain will be written as

$$\epsilon_{kl} = \frac{1}{2}(\partial v_k / \partial x_l + \partial v_l / \partial x_k) = \epsilon_{kl}^{(0)} + e_{kl}^{(m)}x_m + \dots \quad (6)$$

Here x_m is written as a general symbol for x, y, z and summation over subscripts occurring twice is implied. $e_{kl}^{(m)}$ is the strain that would result from a homogeneous stress $p^{(m)}$. If a similar power series for the displacement \mathbf{v} is used, the equations (6) uniquely determine the terms quadratic in x, y, z of that series. One easily checks the validity of

$$v_m = v_m^{(0)} + v_m^{(k)}x_k + [e_{km}^{(l)} - \frac{1}{2}e_{kl}^{(m)}]x_kx_l + \dots \quad (7)$$

Inserting (7) into (4) we find

$$(\omega/ac^2)dA/dl = b'_m(b'_kb'_l + d'_kd'_l)e_{kl}^{(m)} - 2b'_kd'_le_{kl}^{(m)}. \quad (8)$$

We have not yet specified the directions of the x, y and z axes. From what follows it is of advantage to take the z axis perpendicular to the slice in the point Q . The boundary conditions for the stress in a thin slice then require that p_{zx}, p_{zy} and p_{zz} and thus also $p_{zx}^{(k)}, p_{zy}^{(k)}$ and $p_{zz}^{(k)}$ are zero. Furthermore we shall argue later that if the bending moment is applied in a symmetrical way on a specimen of symmetrical shape, so that Q can be chosen in a point that shows symmetry with respect to inversion in the plane of the specimen, $p^{(x)}$ and $p^{(y)}$ also vanish. For such a choice of Q , only $e^{(z)}$ occurs in (8) and it can be calculated from the remaining stress components $p_{xx}^{(z)}, p_{xy}^{(z)}, p_{yy}^{(z)}$. A further simplification is obtained if one chooses the x and y axes in the directions of the normal stresses contained in $p^{(z)}$, *i.e.* so that $p_{xy}^{(z)} = 0$.

It is of some interest to consider the shape of the surface of the slice near Q . It is given by v_z as a quadratic function of x and y . Taking $m = z$ in equation (7) and putting $e^{(x)} = e^{(y)} = 0$ one finds

$$v_z = -\frac{1}{2}x_kx_l e_{kl}^{(z)} \quad (k, l \neq z). \quad (9)$$

Our choice $p_{xy}^{(z)} = 0$ does not necessarily imply $e_{xy}^{(z)} = 0$. Therefore, the geometrical direction of bending in Q does not necessarily coincide with the directions of normal stresses $p_{xx}^{(z)}$ and $p_{yy}^{(z)}$. Also, even for a symmetrical bending apparatus, neither of these directions

can necessarily be directly inferred from the symmetry of the experimental set-up.

Transformations

Expression (8) can be expressed in terms of p with the aid of

$$e = sp \quad (10)$$

where s is the tensor of the elastic compliance. The calculations are complicated by the fact that the components of s are only simple in a system of cubic axes, a, b , and c . Since in (8) we also need the x, y and z components of the vectors \mathbf{b}' and \mathbf{d}' we shall introduce three systems of axes:

- The x, y, z (stress-) system
for which subscripts k, l, m, n are reserved.
- The a, b, c (crystal-) system
for which subscripts g, h, i, j are reserved.
- The ξ, η, ζ (X-ray-) system
for which subscripts λ, μ, ν, τ are reserved.

The η axis is chosen in the \mathbf{b}' direction, the ζ axis in the \mathbf{d}' direction. In order to restrict the number of symbols, all physical vectors or tensors, if represented in different systems, will be distinguished by the use of different types of subscripts only.

Summation over subscripts occurring twice only will always be implied. The orthogonal transformations A and B relate the systems:

$$x_k = A_{kg}x_g; \quad x_k = B_{k\lambda}x_\lambda. \quad (11)$$

Vector components transform as (11), tensors such as e and p as

$$e_{kl} = A_{kg}A_{lh}e_{gh}. \quad (12)$$

In order to evaluate the components of s in the stress (x, y, z) system, we write s as the sum of an isotropic part I , which has the same appearance in all coordinate systems, and a part K , which is typical of the cubic elastic anisotropy and which looks simple in the a, b, c system of cubic axes only (Table 1):

$$K_{ab,ab} = K_{bc,bc} = K_{ca,ca} = K, \quad (13)$$

all other components zero.

Table 1. *The tensor s , in the cubic system of axes*

The part I is invariant for coordinate transformation. (Remember the factor $\frac{1}{2}$ in the definition of the strain.)

aa	I_1	I_2	I_2			
bb	I_2	I_1	I_2			
cc	I_2	I_2	I_1			
ab				$I_1 - I_2 + K$		
bc					$I_1 - I_2 + K$	
ca						$I_1 - I_2 + K$

It follows that

$$e_{kl} = \left(I_{kl, mn} + K \sum_{g \neq h} A_{kg} A_{lh} A_{mg} A_{nh} \right) p_{mn} . \quad (14)$$

Rewriting the restricted summation as an unrestricted summation minus a sum with $g=h$ we have

$$s_{kl, mn} = I_{kl, mn} + K \delta_{km} \delta_{ln} - K \sum_g A_{kg} A_{lg} A_{mg} A_{ng} . \quad (15)$$

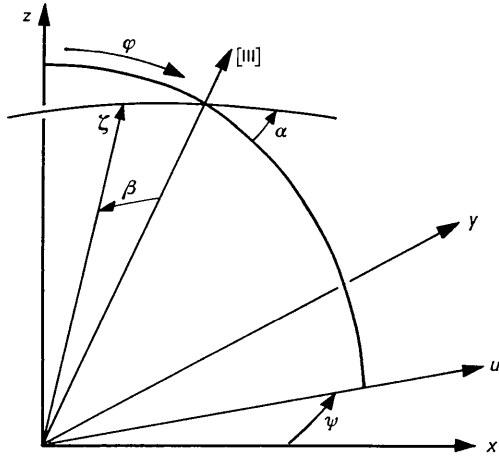


Fig. 2. The Z axis is perpendicular to the slice. Orientation of the [111] axis is shown. The X-ray propagates anomalously in the ζ direction in the (220) plane through the [111] axis.

For the evaluation of (8) we want the components of A and B in terms of angles. Fig. 2 shows that the

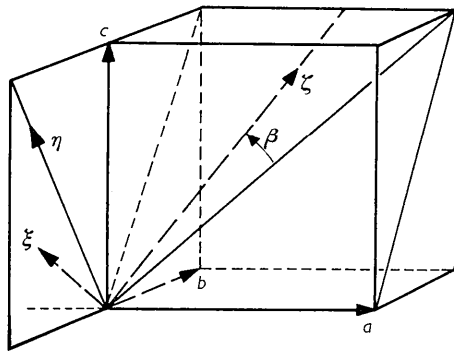


Fig. 3. Orientation of the (ξ, η, ζ) system with respect to the cubic axes (a, b, c) .

[111] axis of the crystal is assumed to make an angle φ with the z axis in a plane (the $z-u$ plane) that makes an angle ψ with the $x-z$ plane. The (220) plane, in which \mathbf{d} lies, makes an angle α with the $z-u$ plane. The angle β , also given in Fig. 3 that shows the cubic axes, is the angle between the ζ direction ($=\mathbf{d}'$ direction) and the [111] axis. Then we have

$$\begin{aligned} B_{x\xi} &= \cos \beta (\sin \psi \sin \alpha - \cos \psi \cos \varphi \cos \alpha) \\ &\quad - \sin \beta \cos \psi \sin \varphi \\ B_{x\eta} &= \sin \psi \cos \alpha + \cos \psi \cos \varphi \sin \alpha \\ B_{x\zeta} &= \sin \beta (\sin \psi \sin \alpha - \cos \psi \cos \varphi \cos \alpha) \\ &\quad + \cos \beta \cos \psi \sin \varphi \\ B_{y\xi} &= -\cos \beta (\sin \psi \sin \alpha + \sin \psi \cos \varphi \cos \alpha) \\ &\quad - \sin \beta \sin \psi \sin \varphi \\ B_{y\eta} &= -\cos \psi \cos \alpha + \sin \psi \cos \varphi \sin \alpha \\ B_{y\zeta} &= -\sin \beta (\cos \psi \sin \alpha + \sin \psi \cos \varphi \cos \alpha) \\ &\quad + \cos \beta \sin \psi \sin \varphi \\ B_{z\xi} &= -\sin \beta \cos \varphi + \cos \beta \sin \varphi \cos \alpha \\ B_{z\eta} &= -\sin \varphi \sin \alpha \\ B_{z\zeta} &= \cos \beta \cos \varphi + \sin \beta \sin \varphi \cos \alpha . \end{aligned} \quad (16)$$

From these formulae one obtains A_{ka} from $B_{k\xi}$ by putting $\sin \beta = -\sqrt{2/3}$, $\cos \beta = \sqrt{1/3}$, A_{kb} and A_{kc} from A_{ka} by writing respectively $\alpha + 2\pi/3$ and $\alpha - 2\pi/3$ instead of α .

We are now ready to write down (8) in terms of the components of A and B ; if b' and d' are the absolute values of the vectors \mathbf{b}' and \mathbf{d}' and the Bragg angle Θ is given by $\tan \Theta = b'/d'$ we have ($m=z$ only):

$$\begin{aligned} (\omega/ac^2 b'^3) dA/dl &= (s_{kl, xx} p_{xx}^{(z)} + s_{kl, yy} p_{yy}^{(z)}) \\ &\quad \times [B_{z\eta} B_{k\eta} B_{l\eta} + \cotan^2 \Theta (B_{z\eta} B_{k\zeta} B_{l\zeta} - 2B_{z\zeta} B_{k\zeta} B_{l\eta})] . \end{aligned} \quad (17)$$

Evaluation when φ is zero or small

If the [111] axis is perpendicular to the surface, $\varphi=0$ and we have, if $\Sigma(k, l, m, n) = \sum_g A_{kg} A_{lg} A_{mg} A_{ng}$

$$\begin{aligned} \Sigma(x, x, x, x) &= \Sigma(y, y, y, y) = 1/2 \\ \Sigma(x, y, x, x) &= \Sigma(x, y, y, y) = 0 \\ \Sigma(y, y, x, x) &= \Sigma(x, x, y, y) = 1/6 \\ \Sigma(x, z, x, x) &= -\Sigma(x, z, y, y) = (\sqrt{2}/6) \cos 3(\alpha + \psi) \\ \Sigma(y, z, x, x) &= -\Sigma(y, z, y, y) = (\sqrt{2}/6) \sin 3(\alpha + \psi) . \end{aligned} \quad (18)$$

It follows that the expression in equation (17) is

$$\begin{aligned} (17) &= 2 \cotan^2 \Theta \cos \beta \cos(\alpha + \psi) \sin(\alpha + \psi) \\ &\quad \times (p_{xx}^{(z)} - p_{yy}^{(z)}) [(I_1 - I_2 + 2K/3) \sin \beta - (K\sqrt{2}/3) \cos \beta] . \end{aligned} \quad (19)$$

Thus if a (220) plane is parallel to a direction of stress ($\cos(\alpha + \psi)$ or $\sin(\alpha + \psi)$ zero) no reduction of intensity on bending will be observed for X-rays anomalously transmitted along that plane. For other values of $\alpha + \psi$ there will be a decrease on bending, except for that direction of propagation, *i.e.* that value of β for which the factor in the square brackets in (19) vanishes. In that case the remaining intensity distribution shows the apparent threefold symmetry

observed by van Bommel. We shall return to this point in the discussion.

For $\varphi=0$ it also follows that

$$\begin{aligned} e_{xx} &= (I_1 + K/2)p_{xx}^{(z)} + (I_2 - K/6)p_{yy}^{(z)} \\ e_{yy} &= (I_2 - K/6)p_{xx}^{(z)} + (I_1 + K/2)p_{yy}^{(z)} \\ e_{xy} &= 0 \end{aligned} \quad (20)$$

from which the shape of the surface can be calculated by (9). It is seen that for $\varphi=0$ the geometrical direction of bending in our point Q coincides with the directions of stress.

If φ is small, we have to the first order in φ :

$$\begin{aligned} e_{xy} &= (K\sqrt{2}/6) \sin \varphi \cdot p_{yy}^{(z)} \\ &\times [\sin 3(\alpha + \psi) \cos \psi + 3 \cos 3(\alpha + \psi) \sin \psi] \\ &- (K\sqrt{2}/6) \sin \varphi \cdot p_{xx}^{(z)} \\ &\times [\cos 3(\alpha + \psi) \sin \psi + 3 \sin 3(\alpha + \psi) \cos \psi] \end{aligned} \quad (21)$$

and the small angle between the direction of stress and the direction of bending is $e_{xy}(I_1 - I_2 + 2K/3)^{-1}$.

For small φ it is of some interest to evaluate (17) for the case $\sin(\alpha + \psi) = 0$, or $\cos(\alpha + \psi) = 0$. We give the results for the case in which $p_{xx}^{(z)}$ vanishes. If $\sin(\alpha + \psi) = 0$

$$\begin{aligned} (17) &= -\delta(I_1 + K/2)p_{yy}^{(z)} - \delta \cotan^2 \Theta p_{yy}^{(z)} \\ &\times [2I_1 - I_2 + K/3 - K\sqrt{2} \cos \beta \sin \beta \\ &- 2 \sin^2 \beta (I_1 - I_2 + K/4)]. \end{aligned} \quad (22)$$

If $\cos(\alpha + \psi) = 0$

$$\begin{aligned} (17) &= -\delta(I_1 - K/6)p_{yy}^{(z)} - \delta \cotan^2 \Theta p_{yy}^{(z)} \\ &\times [I_2 - K/3 + (K\sqrt{2}/3) \cos \beta \sin \beta \\ &+ \sin^2 \beta (I_1 - I_2 + 5K/6)]. \end{aligned} \quad (23)$$

In both cases the effect is proportional to $\delta = \sin \alpha \sin \varphi$, being the angle between the (220) plane and the normal to the surface. Case I applies to the case discussed in a previous paper (Penning & Polder, 1961), and it may serve to correct equation (34) of that paper for the effect of cubic anisotropy. Since φ is small one puts $\cos 2\varphi = 1$ in that equation. The anisotropy will then be accounted for if one replaces $1 + \nu = 1 - I_2/I_1$ by $1 + \nu - K/(6I_1)$. To prove this, one has to use the identity $R^{-1} = (I_1 + K/2)p_{yy}^{(z)}$, which follows from (20).

The stress pattern

We assume that the bending moment is applied in a symmetrical manner on a symmetrical specimen, so that Q can be located in a point, fixed to the specimen, that shows symmetry with respect to the inversion operation ($x \rightarrow -x$, $y \rightarrow -y$, $z \rightarrow z$). If the elastic tensor s is invariant also for this operation (which implies invariance for $z \rightarrow -z$, since s is in-

variant for $x \rightarrow -x$, $y \rightarrow -y$, $z \rightarrow -z$) the solution of the bending problem must be symmetrical for ($x \rightarrow -x$, $y \rightarrow -y$), i.e. $p_{xx}^{(k)}$, $p_{xy}^{(k)}$, and $p_{yy}^{(k)}$ are all zero for $k=x$ or y in the point Q , while $p^{(z)}$ survives.

This, together with the boundary condition $p_{zk} = 0$, gives the stress field assumed to be present in our paper. However, the tensor s is not invariant for ($x \rightarrow -x$, $y \rightarrow -y$), since according to (15) the term $\Sigma(klmn)$ is not, if the set $(klmn)$ contains the subscript z an odd number of times.

Let us, therefore, for the time being, ignore these terms and assume that we have solved the elastic problem for a hypothetical material characterized by an s tensor without the odd terms. The stress tensor will then be of the type assumed in this paper, i.e. it contains only $p_{xx}^{(z)}$ and $p_{yy}^{(z)}$ in Q . If the stress tensor is now thought to be kept fixed, the odd terms in s will, in the real material, produce an additional strain, which, since $p_{zk} = 0$, will everywhere consist of ϵ_{xz} and ϵ_{yz} only. The additional strain can be described by an additional displacement in the plane of the specimen and is proportional to z everywhere. The additional displacement does not change the shape of the bent surface, nor that of the specimen and therefore does not interfere with the boundary conditions of the elastic problem, at least not for a thin specimen. Therefore we conclude that the stress field for the real material will be the same as that for the hypothetical material and of the type as assumed in discussing the elastic deformation.

Discussion

In the experiments by van Bommel a point source of X-rays is located at a distance u from the front surface of a germanium slice which has the [111] axis perpendicular to the surface. A photographic plate, parallel to the surface of the specimen, is present at a distance l from the back surface of the slice.

The distance between source and plate is $u + w + l$, if w is the thickness of the specimen. We define an X, Y system of axes on the plate, the origin being the geometrical projection of the source on the plate, the X axis being parallel to a given (220) plane through the [111] axis. An X-ray that is anomalously transmitted through the crystal having a ζ direction defined by the angle β as in Fig. 3, will arrive on the plate with the X coordinate given by

$$X/(u + w + l) = \tan \beta. \quad (24)$$

The total length of the projection of the X-ray path on the (220) plane is therefore $(u + w + l)/\cos \beta$. Between the source and the front surface the X-ray travels at the Bragg angle Θ with the (220) plane; in the crystal it travels parallel to that plane; at the back surface it splits into a beam at an angle Θ (the transmitted ray) and one at an angle $-\Theta$ (the

reflected ray). The Y coordinates on the plate of these beams are then given respectively by:

$$Y = (u \pm l) \tan \Theta / \cos \beta. \quad (25)$$

Eliminating β from (24) and (25) we have

$$\tan^2 \beta = X^2 / (u + w + l)^2 = -1 + Y^2 \cot^2 \Theta / (u \pm l)^2. \quad (26)$$

Equation (26) defines four curved lines on the plate, two being caused by the transmitted and reflected beams we have described, the other two being caused by an X-ray emerging from the source at an angle $-\Theta$ with the (220) plane. Actually one finds three sets of four lines on the plate as there are three (220) planes through our [111] axis. The picture shows sixfold symmetry.

If $u=0$, three sets of two lines will appear. We shall consider what happens in this case if the crystal is bent in such a way that none of the three (220) planes is perpendicular or parallel to the direction of stress. According to equation (19) anomalous transmission will survive only for rays with a β value given by

$$\tan \beta = K \sqrt{2/3} (I_1 - I_2 + 2K/3). \quad (27)$$

Let us insert numerical values for germanium. We have for Cu $K\alpha$ radiation $\tan \Theta = 0.415$, $I_2/I_1 = -0.273$ and $K/I_1 = -0.508$ as follows from the elastic data.* Thus $\tan \beta = -0.256$. Neglecting w with respect to l in (26) we find two values for Y and one for X (cf. equation (24)) such that $Y/X = \pm 1.67$. Since $\arctan(1.67) = 59^\circ$ the surviving intensity, accidentally, occurs very nearly at the intersection of the lines resulting from different (220) planes (Fig. 4). The resulting picture now shows (apparent) threefold symmetry. The threefold symmetry is only apparent, since, if one of the three planes is either perpendicular

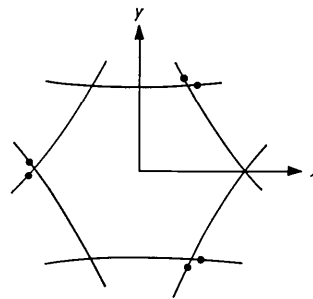


Fig. 4. Principal features of the picture of the photographic plate in van Bommel's experiment.

or parallel to the stress direction, the intensity of the corresponding pair of lines will not decrease, while for the other two pairs only the spots with the correct β value will survive.

The major consequences of the theory

Surviving pairs of lines (or four lines if $u \neq 0$) for two directions of stress, surviving intensity near the intersections with threefold symmetry for other directions of stress, and the sign of β , have all been found by van Bommel (1964). In particular the sign of β is uniquely negative and it has been verified to be correct by the inspection of the relation between the observed threefold symmetry and the crystal orientation.

The good agreement between theory and experiment shows the usefulness of the theoretical approach as given by Penning & Polder (1961) even in quite complicated cases.

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* The conventional elastic constants are:

$$S_{11} = I_1, \quad S_{12} = I_2, \quad S_{44} = 2(I_1 - I_2 + K).$$