In Table 4 theoretical values in Tables 1 and 2 are compared with experimental values of V^i_g. Agreement is satisfactory in most cases. Exceptions at V^i_0 may be due to theoretical assumptions about the minimum scattering wave vector while slight deviations at V^i_g may be partly explained on the experimental side, where evaluation is rendered difficult by complications such as, for instance, many-beam effects.

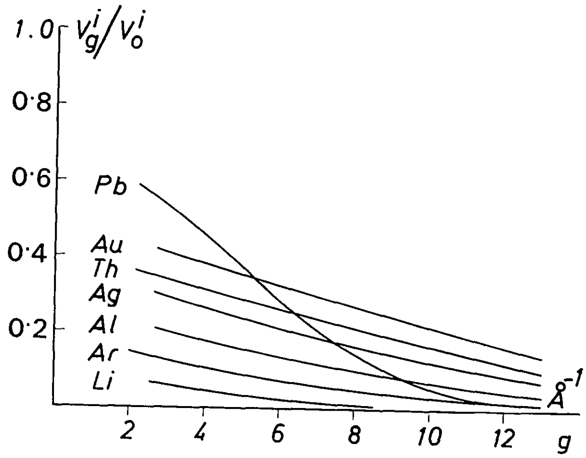

Fig. 6. V^i_g/V^i_0 as a function of g for some crystals.

References

Bethe, H. A. (1928). *Ann. Phys.* **87**, 55.
Ferrell, R. A. (1956). *Phys. Rev.* **101**, 554.
Goodman, P. & Lehmpfuhl, G. (1967). *Acta Cryst.* **22**, 14.
Goringe, M. J. & Whelan, M. J. (1966). *Electron Microscopy*, Vol. I, p.49. Tokyo: Maruzen.
Graff, K. & Gaukler, K. M. (1969). To be published.
Hall, C. R. & Hirsch, P. B. (1965). *Proc. Roy. Soc.* A**286**, 158.
Hashimoto, H. (1964). *J. Appl. Phys.* **35**, 277.
Herman, F. & Skillman, S. (1963). *Atomic Structure Calculations*. Englewood Cliffs: Prentice Hall.
Humphreys, C. J. & Hirsch, P. B. (1968). *Phil. Mag.* **18**, 115.
International Tables for X-ray Crystallography (1962). Vol. III, p. 233. Birmingham: Kynoch Press.
Lenz, F. (1954). *Z. Naturforsch.* A**9**, 185.
Metherell, A. J. F. & Whelan, M. J. (1967). *Phil. Mag.* **15**, 755.
Meyer-Ehmsen, G. (1969). *Z. Phys.* **218**, 352.
Ohtsuki, Y. H. (1966). *J. phys. Soc. Japan*, **21**, 2300.
Radi, G. (1968). *Z. Phys.* **212**, 146; **213**, 244.
Yoshioka, H. (1957). *J. phys. Soc. Japan*, **12**, 618.
Yoshioka, H. & Kainuma, Y. (1962). *Proc. Int. Conf. Magn. Cryst. Kyoto*, 1961; *J. phys. Soc. Japan*, **17B-II**, 134.
Watanabe, H. (1965). *Jap. J. Appl. Phys.* **4**, 384.
Whelan, M. J. (1965*a*). *J. Appl. Phys.* **36**, 2099.
Whelan, M. J. (1965*b*). *J. Appl. Phys.* **36**, 2103.

Acta Cryst. (1969). A**25**, 56

The Dynamical Scattering Amplitude of an Imperfect Crystal

By Masao Kuriyama

Institute for Materials Research, National Bureau of Standards, Washington, D.C. 20234, *U.S.A.*

(*Received* 21 *February* 1969)

A formal expression for the X-ray dynamical scattering amplitude of an imperfect crystal is obtained. The resultant expression includes the dynamical line broadening effect on the diffracted X-rays caused by imperfections. The effects due to absorption in the crystal are also taken into account.

1. Introduction

In studying the problems of diffraction by crystals it is desirable to have a dynamical solution for diffracted beams because, even under a single Bragg condition, there are strong interactions between the crystal electrons and the beams. When the crystal is perfect, one uses the two-wave approximation to derive an approximate dynamical solution for a single Bragg reflection. When an incident beam satisfies several Bragg conditions simultaneously, one needs to employ 'more than two'-wave approximations which are sometimes only solvable by numerical computations.

There is no true dynamical theory for diffraction unless the multiple interaction is correctly treated. Since difficulty is encountered in obtaining dynamical solutions for a perfect crystal, greater difficulty is expected in seeking completely dynamical solutions for an imperfect crystal.

In electron diffraction where the multiple scattering is essential, a formal theory of dynamical diffraction has been formulated by Niehrs (1959*a*,*b*) and Fujimoto (1959, 1960). In this theory the scattering amplitude is completely dynamical in form. In practice, it is admittedly tedious to calculate the scattering amplitude to a great degree of accuracy. Nevertheless this amplitude can be calculated to a far higher degree of accuracy than the two-or many-wave approximations. This is possible because the two or the solvable many-wave approximations are the zero order approximations in this scattering amplitude. In this sense the scattering amplitude is useful although this is indeed formal.

By contrast, in X-ray diffraction from a perfect crystal, a single Bragg reflection condition is valid in general and the many-beam approximations are not indispensable. Therefore, there has not been so far an immediate need for a completely dynamical expression for the scattering amplitude in X-ray diffraction. However, when one considers the X-ray diffraction problems for an imperfect crystal the situation becomes entirely different. Even though a single Bragg reflection condition is satisfied by an incident wave, the diffracted wave can propagate in any direction. In reality, it propagates mostly in directions around the transmitted and the Bragg diffracted directions (Kuriyama, 1968*a*,*b*). In other words, the diffracted (including the transmitted direction) beams have line broadening around the propagation directions expected from a perfect crystal. This situation implies that there are many beams simultaneously scattered from the imperfect crystal. If one wishes to have a dynamical theory for an imperfect crystal, then one has to seek as good a solution for a multiple interaction problem as in electron diffraction.

In the present paper a formal solution for dynamical diffraction from an imperfect crystal is obtained. Unlike the electron diffraction theories mentioned before, the present formulation is derived for a crystal in which there is absorption of the scattered X-rays. In an imperfect crystal it is always essential to take into account this effect.

2. A formal expression for the dynamical scattering amplitude

Two basic equations for X-ray diffraction by a crystal are the scattering amplitude and the photon Green's function equations. The scattering amplitude for an X-ray beam striking a crystal at **R** with momentum **k** to make a transition to the state of momentum **k**′ emerging at **R**′ is given (Ashkin & Kuriyama, 1966) by

$$\langle \mathbf{k}'\mathbf{R}'|S|\mathbf{k}\mathbf{R}\rangle = \int d^3p' \int d^3p A^*(\mathbf{k}',\mathbf{p}';\mathbf{R}')S(\mathbf{p}',\mathbf{p})A(\mathbf{k},\mathbf{p};\mathbf{R}), \tag{2·1}$$

where A is the Fourier transform of the free photon wave packet depending on a parameter **R** which indicates the spatial location for the maximum intensity. Throughout this paper, only a scalar field is treated in order to avoid unnecessary complications. The thory for X-ray fields is the same except for the polarization factors. The quantity $S(\mathbf{p}',\mathbf{p})$ is the scattering matrix element and is given (Kuriyama, 1967*a*,*b*) by

$$S(\mathbf{p}',\mathbf{p}) = \delta(\mathbf{p}' -- \mathbf{p}) + i \int_{\text{crystal}} d^4x_1 \int d^4x_2 \chi^*_{\mathbf{p}'}(x_1)\chi_{\mathbf{p}}(x_2) \int$$

$$\times \frac{d\omega}{2\pi} \int \frac{d^3k_1}{(2\pi)^3} \int \frac{d^3k_2}{(2\pi)^3} [(k_1^2-\omega^2)(k_2^2 -\omega^2)D(\mathbf{k}_1,\mathbf{k}_2;\omega) - 4\pi(2\pi)^3(k_2^2-\omega^2)\delta(\mathbf{k}_1 - \mathbf{k}_2)] \times \exp[i\mathbf{k}_1\mathbf{r}_1 - i\mathbf{k}_2\mathbf{r}_2 - i\omega(t_1-t_2)], \tag{2·2}$$

where

$$\chi_p(x) = [2(2\pi)^3 4\pi|\mathbf{p}|]^{1/2} \exp[i(\mathbf{p}\,.\,\mathbf{r} - |\mathbf{p}|t)]. \tag{2·3}$$

The quantity $D(\mathbf{k}_1,\mathbf{k}_2;\omega)$ is the Fourier transform of the photon Green's function and satisfies the photon Green's function equation (Kuriyama, 1967*a*,*b*):

$$(k_1^2-\omega^2)D(\mathbf{k}_1,\mathbf{k}_2;\omega) - \int \frac{d^3p}{(2\pi)^3} \Gamma(\mathbf{k}_1,\mathbf{p};\omega)D(\mathbf{p},\mathbf{k}_2;\omega) = 4\pi(2\pi)^3\delta(\mathbf{k}_1-\mathbf{k}_2), \tag{2·4}$$

where $\Gamma(\mathbf{k}_1,\mathbf{k}_2;\omega)$ is the Fourier transform of the generalized polarizability of the crystal.

When the atoms in the crystal are displaced from their positions in the perfect crystal, the Fourier transform of the generalized polarizability is given (Kuriyama, 1967*a*) by

$$\Gamma(\mathbf{k}_1,\mathbf{k}_2;\omega) = g(\mathbf{k}_1-\mathbf{k}_2)\gamma(\mathbf{k}_1,\mathbf{k}_2;\omega), \tag{2·5}$$

where $g(\mathbf{k}_1-\mathbf{k}_2)$ is the geometrical structure factor for the crystal and is defined by

$$g(\mathbf{k}_1-\mathbf{k}_2) = V_c \sum_{\mathbf{l}} \exp[-i(\mathbf{k}_1-\mathbf{k}_2)\mathbf{R}_{\mathbf{l}}]. \tag{2·6}$$

The Fourier transform of the polarizability of 'atomic' electrons in the unit cell is denoted by $\gamma(\mathbf{k}_1,\mathbf{k}_2;\omega)$. The quantity V_c is the unit-cell volume and $\mathbf{R}_{\mathbf{l}}$ the atomic position displaced by $\mathbf{u}_{\mathbf{l}}$ from the ideal lattice site **l**. The crystal contains N atoms.

For the present purpose it may be assumed without loss of generality (see 3) that the atomic displacement can be expressed by

$$\mathbf{u}_{\mathbf{l}} = \mathbf{A}_{\mathbf{q}} \sin(\mathbf{q}\,.\,\mathbf{l} - \Phi_{\mathbf{q}}). \tag{2·7}$$

Then, (2·6) reduces to

$$g(\xi) = NV_c \sum_{n=-\infty}^{+\infty} C_n(\xi)\Delta^{(3)}(\xi + n\mathbf{q}), \tag{2·8}$$

where

$$C_n(\xi) = J_n(\xi\,.\,\mathbf{A}_{\mathbf{q}}) \exp[in\Phi_{\mathbf{q}}], \tag{2·9}$$

and $\Delta^{(3)}$ is the generalized Kronecker delta, being unity when $\xi + n\mathbf{q}$ is equal to a reciprocal lattice vector **K** defined in the perfect reference crystal, and otherwise being almost zero. When the size of the crystal is infinite, this function becomes the delta function as follows:

$$NV_c\Delta^{(3)}(\xi + n\mathbf{q}) = (2\pi)^3 \sum_{\mathbf{K}} \delta(\xi + n\mathbf{q} - \mathbf{K}). \tag{2·10}$$

To simplify notations it is assumed further that

$$\gamma(\mathbf{k}_1,\mathbf{k}_2;\omega)=\gamma(\mathbf{k}_1-\mathbf{k}_2;\omega)\,. \tag{2·11}$$

The Fourier transform of the generalized polarizability for an infinite crystal is then written

$$\Gamma(\mathbf{k}_1,\mathbf{k}_2;\omega)=(2\pi)^3\sum_{\mathbf{K}}\sum_{n}\gamma_n(\mathbf{k}_1-\mathbf{k}_2)\delta(\mathbf{k}_1-\mathbf{k}_2+n\mathbf{q}-\mathbf{K})\,, \tag{2·12}$$

where

$$\gamma_n(\mathbf{k}_1-\mathbf{k}_2)=C_n(\mathbf{k}_1-\mathbf{k}_2)\gamma(\mathbf{k}_1,\mathbf{k}_2;\omega)\,. \tag{2·13}$$

By substitution of (2·12), the photon Green's function equation (2·4) reduces to

$$(k_1^2-\omega^2)D(\mathbf{k}_1,\mathbf{k}_2;\omega)-\sum_{\mathbf{J}}\sum_{n}\gamma_n(\mathbf{J}-n\mathbf{q})D(\mathbf{k}_1+n\mathbf{q}-\mathbf{J},\mathbf{k}_2;\omega)=4\pi(2\pi)^3\delta(\mathbf{k}_1-\mathbf{k}_2)\,, \tag{2·14}$$

where, instead of **K**, **J** is used to represent a reciprocal lattice vector. Equation (2·14) gives a set of inhomogeneous simultaneous equations since (2·14) is valid for any value of $\mathbf{k}_1$ (for instance, $\mathbf{k}_1=\bar{\mathbf{k}}_1+m\mathbf{q}-\mathbf{I}$, where m is an integer and **I** is a reciprocal lattice vector). This set of simultaneous equations can therefore be written in a matrix form

$$\mathbf{MD}=\mathbf{E}\,, \tag{2·15}$$

where **D** and **E** are column matrices given by

$$D_{n\mathbf{J}}=D(\mathbf{k}_1+n\mathbf{q}-\mathbf{J},\mathbf{k}_2;\omega) \tag{2·16}$$

and

$$E_{n\mathbf{J}}=4\pi(2\pi)^3\delta(\mathbf{k}_1+n\mathbf{q}-\mathbf{J}-\mathbf{k}_2)\,. \tag{2·17}$$

The matrix **M** is given by

$$[M(\mathbf{k}_1;\omega)]_{m\mathbf{I},\,n\mathbf{J}}=[(\mathbf{k}_1+m\mathbf{q}-\mathbf{I})^2-\omega^2]\delta_{m,\,n}\delta_{\mathbf{I},\mathbf{J}}-\gamma_{n-m}(\mathbf{J}-\mathbf{I}-(n-m)\mathbf{q})\,. \tag{2·18}$$

The solution of equation (2·15) is thus given by

$$\mathbf{D}=\mathbf{M}^{-1}\,.\,\mathbf{E}\,, \tag{2·19}$$

where $\mathbf{M}^{-1}$ is the inverse matrix of **M**. In components (2·19) is written

$$D_{m\mathbf{I}}=4\pi(2\pi)^3\sum_{n}\sum_{\mathbf{J}}[\mathbf{M}^{-1}(k_1;\omega)]_{m\mathbf{I},\,n\mathbf{J}}\delta(\mathbf{k}_1+n\mathbf{q}-\mathbf{J}-\mathbf{k}_2)\,. \tag{2·20}$$

This is a set of dynamical solutions of the photon Green's function for the imperfect crystal of infinite size. The same basic principle as in the theory for a perfect crystal (Ashkin & Kuriyama, 1966) is adopted here in calculating the scattering amplitude of a finite crystal. The principle is that an accurate treatment of the scattering by a finite crystal should be obtained by using the dynamical solution of the photon Green's function for an infinite crystal in conjunction with the modified 'contraction' formula of the scattering amplitude.

The scattering matrix element can now be calculated by (2·2) with $D(\mathbf{k}_1,\mathbf{k}_2;\omega)$ substituted by $D_{o\mathbf{O}}$ in (2·20). The scattering matrix element will be evaluated for an imperfect crystal plate of limited dimension in one direction and of infinite dimension in the remaining two orthogonal directions. For convenience the origin of the coordinate system is chosen on the entrance face of the crystal and the z axis along the direction of finite extent of the crystal. The crystal occupies the region between $z=0$ and $z=L$, where L is the crystal thickness. The projection of a vector onto the crystal surface is described by a subscript t. The Laue geometry is considered explicitly. Furthermore, it is assumed that the reciprocal lattice vectors **I** and **J** belong to a set of the reciprocal lattice points which nearly satisfy Bragg conditions simultaneously. For such **I** or **J** it follows that $k_{1,z}+mq_z-I_z\simeq p'_z$.*

With this choice of coordinates, (2·2) reduces to

$$S(\mathbf{p}',\mathbf{p})=\delta(\mathbf{p}'-\mathbf{p})+\frac{i}{2|\mathbf{p}|}\delta(|\mathbf{p}'|-|\mathbf{p}|)\sum_{n,\,\mathbf{J}}\delta(\mathbf{p}_t-n\mathbf{q}_t+\mathbf{J}_t-p'_t)\times[\{1+\exp[i(p_z-nq_z+J_z-p'_z)L]\}t_o-\exp[-i(nq_z-J_z+p'_z)L]t_+-\exp[ip_zL]t_-]\,, \tag{2·21}$$

where

$$t_\pm=(2p_z)\int_{-\infty}^{+\infty}\frac{\mathrm{d}k_z}{2\pi}\{(2p'_z)[\mathbf{M}^{-1}(\mathbf{p}'_z,k_z-nq_z+J_z;|\mathbf{p}|)]_{o\mathbf{O},n\mathbf{J}}-(k_z-p_z)^{-1}\delta_{n\mathbf{J},o\mathbf{O}}\}\exp[\pm ik_zL]\,, \tag{2·22}$$

and t_o is given by (2·22) with $L=0$. The integrand of t_o decreases more rapidly than $(k_z)^{-1}$ as k_z approaches infinity. Therefore, the integrals t_o and $t_\pm$ are given by their residues.

To evaluate the residues, it is convenient to rewrite the matrix **M**, (2·18), in such a way that the matrix element is given by a sum of two terms, one of which is independent of k_z. For the reciprocal lattice vectors **I** and **J** of interest,* the matrix element of **M** is given by

$$[\mathbf{M}(\mathbf{p}'_t,k_z-nq_z+J_z;|\mathbf{p}|)]_{m\mathbf{I},n\mathbf{J}}=[\mathbf{M}_o(\mathbf{p}')]_{m\mathbf{I},n\mathbf{J}}+2p'_z(k_z-p'_z)\delta_{m\mathbf{I},n\mathbf{J}}\,, \tag{2·23}$$

where

$$[\mathbf{M}_o(\mathbf{p}')]_{m\mathbf{I},n\mathbf{J}}=[(\mathbf{p}'+m\mathbf{q}-\mathbf{I})^2-(\mathbf{p}')^2]\delta_{m\mathbf{I},n\mathbf{J}}-\gamma_{n-m}(\mathbf{J}-\mathbf{I}-(n-m)\mathbf{q})\,. \tag{2·24}$$

The inverse matrix $\mathbf{M}^{-1}$ is now written

---

* To avoid unnecessary mathematical complications, the nearly symmetrical reflection condition is being treated. For an asymmetrical reflection, a transformation on **M** is needed, resulting in $\mathbf{M}_o$, (2·24), replaced by $\mathbf{M}_o\Theta^{-2}$, where $\Theta_{m\mathbf{I},n\mathbf{J}}=[(p'_z-mq_z+I_z)/p'_z]^{1/2}\delta_{m\mathbf{I},n\mathbf{J}}$.

$$\mathbf{M}^{-1}=(\mathbf{M}_o+2p'_z(k_z-p'_z)\mathbf{I})^{-1}$$
$$=\sum_{m=o}^{+\infty}\frac{(-\mathbf{M}_o)^m}{(2p'_z)^{m+1}(k_z-p'_z)^{m+1}}\,, \quad (2\cdot25)$$

where $\mathbf{I}$ is the identity matrix. Since $\mathbf{M}_o$ is independent of k_z, the integrals t_o and $t_\pm$ reduce to

$$t_\pm=(2p_z)\exp\left[\pm i(nq_z-J_z)L\right]\sum_m\frac{1}{(2p'_z)^m}\left[(-\mathbf{M}_o)^m\right]_{o\mathbf{O},n\mathbf{J}}$$
$$\times\int\frac{\mathrm{d}k}{2\pi}\left[\frac{1}{(k-p'_z-i\varepsilon)^{m+1}}-\frac{\delta_{m,o}\delta_{n\mathbf{J},o\mathbf{O}}}{k-p_z-i\varepsilon}\right]$$
$$\times\exp\left[\pm\ ikL\right], \quad (2\cdot26)$$

and similarly t_o is given without the exponential factors. Here ε is an infinitesimally small number. These integrals are easily evaluated to give

$$S(\mathbf{p}',\mathbf{p})=\delta(\mathbf{p}'-\mathbf{p})+\frac{i}{2|\mathbf{p}|}\,\delta(|\mathbf{p}'|$$
$$-|\mathbf{p}|)\,\Sigma\,\delta(\mathbf{p}_t-n\mathbf{q}_t+\mathbf{J}_t-\mathbf{p}'_t)$$
$$\times(-i)\,(2p_z)\left[\sum_m\frac{1}{m!}\left[\left(\frac{-i\mathbf{M}_oL}{2p'_z}\right)^m\right]_{o\mathbf{O},n\mathbf{J}}\right.$$
$$\left.-\delta_{n\mathbf{J},o\mathbf{O}}\right]. \quad (2\cdot27)$$

Two useful identity equations are

$$\sum_{m=0}^{\infty}\frac{1}{m!}\mathbf{A}^m=\exp\mathbf{A}\,. \quad (2\cdot28)$$

and

$$\frac{1}{2|\mathbf{p}|}\,\delta(|\mathbf{p}'|-|\mathbf{p}|)\delta(\mathbf{p}'_t-\mathbf{p}_t)=\frac{1}{2p_z}\,\delta(\mathbf{p}'-\mathbf{p})\,. \quad (2\cdot29)$$

Equation (2·27) thus reduces to the desired result†

$$S(\mathbf{p}',\mathbf{p})=(p_z/|\mathbf{p}|)\delta(|\mathbf{p}'|-|\mathbf{p}|)\sum_{n\mathbf{J}}\delta(\mathbf{p}_t-n\mathbf{q}_t+\mathbf{J}_t-\mathbf{p}'_t)$$
$$\times\left[\exp\left\{-i\frac{L}{2p'_z}\mathbf{M}_o(\mathbf{p})\right\}\right]_{o\mathbf{O},n\mathbf{J}}\,. \quad (2\cdot30)$$

3. Conclusion and discussion

In deriving (2·30) several approximations have been used. Among them are (1) that the reciprocal vectors **I** and **J** of our interest should lie very close to the Ewald sphere, and (2) that the polarizability $\gamma(\mathbf{k}_1,\mathbf{k}_2;\omega)$ of the 'atomic' electrons should be independent of $k_{2,z}$. Both of these assumptions are indispensable at present. The assumption that the atomic displacement $\mathbf{u}_l$ is given by (2·7) is not needed at all.

In general, the atomic displacement vectors are given by a superposition of (2·7) over various **q**'s. Although the expression of $g(\mathbf{k}_1-\mathbf{k}_2)$ becomes complicated, it is still true to write $g(\mathbf{k}_1-\mathbf{k}_2)$ in the form shown in (2·8). Any given function $f(x)$ can be defined by

$$f(x)=g_x(y)\delta_{x,y}=\sum_y g_x(y)\delta_{x,y} \quad (3\cdot1)$$

where δ is the Kronecker delta and g_x is a function of y which takes on the value of $f(x)$ at $y=x$ and can be arbitrary elsewhere. This is exactly the form obtained in (2·8) if $n\mathbf{q}$ is considered to be a parameter like y, while **I** and **J** are chosen so that they can satisfy the assumption (1). It is therefore concluded that the final result of $S(\mathbf{p}',\mathbf{p})$ is always valid regardless of the form of $\mathbf{u}_l$.

Since no restrictions have been imposed on the property of the matrix $\mathbf{M}$ (for instance, $\mathbf{M}$ is not necessarily Hermitian), the absorption effect has been taken into account. The scattering amplitude of an imperfect crystal for an incoming wave of finite size (spherical wave) is given by (2·1) with the scattering matrix element (2·30). Since all the dynamical interactions have been built into (2·30), this resultant scattering amplitude is dynamical in form.

When the crystal is perfect, this scattering amplitude becomes identical to the formal dynamical expression given by Niehrs (1959*a*,*b*) and Fujimoto (1959, 1960); it gives nonvanishing values only in the transmitted and the Bragg diffracted directions, and vanishes elsewhere. When the crystal is imperfect, the obtained scattering amplitude gives non-vanishing values not only in the transmitted and Bragg diffracted directions, but also in any direction, because the quantity $n\mathbf{q}$ can be considered to be a continuous variable. This implies that the resultant expression for the scattering amplitude includes the dynamical line broadening effect due to imperfections (Kuriyama, 1967*a*, 1968*a*).

References

Ashkin, M. & Kuriyama, M. (1966). *J. Phys. Soc. Japan*, **21**, 1549.
Fujimoto, F. (1959). *J. Phys. Soc. Japan*, **14**, 1558.
Fujimoto, F. (1960). *J. Phys. Soc. Japan*, **15**, 859.
Kuriyama, M. (1967*a*). *J. Phys. Soc. Japan*, **23**, 1369.
Kuriyama, M. (1967*b*). *Phys. Stat. Sol.* **24**, 743.
Kuriyama, M. (1968*a*). *J. Appl. Phys.* **39**, 2162.
Kuriyama, M. (1968*b*). *J. Phys. Soc. Japan*, **25**, 846.
Niehrs, H. (1959*a*). *Z. Naturforsch.* **14*a***, 504.
Niehrs, H. (1959*b*). *Z. Physik*, **156**, 446.

---

† For an asymmetrical reflection, $\mathbf{M}_o$ is replaced by $\mathbf{M}_o\Theta^{-2}$.