Wilcock (1946) that the layers have stopped on arriving at the side of a trigon. Very probably this is true only when the layers are thicker than a certain value.

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The Equation of Kikuchi Lines on the Basis of the Kikuchi Geometrical Model

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The applicability of the Kikuchi model of the origin of *P* patterns in electron diffraction is discussed. With the use of this model the equation of Kikuchi lines is derived and examples are given of crystallographic measurements carried out with high accuracy by means of this equation.

Introduction

Various electron diffraction patterns for the case of a single crystal have been investigated. These can be conventionally classified into three types: *N*, *L* and *P* (Pinsker, 1949).

Kikuchi (1928) proposed a geometrical model (Fig. 1) which is very simple but seems to be useful for describing the geometry of *P* patterns. Finch, Quarell & Wilman (1935), Finch & Wilman (1936), and Wilman (1948) described some possibilities of this model. In the present paper we give (1) the derivation of the equation of Kikuchi lines for an arbitrary experimental arrangement and (2) some examples of the practical applications of this equation.

Applicability of the Kikuchi model

Using the Kikuchi model we suppose the primary wave to be scattered by the first (upper) part of a thick crystal. The wave packet is obtained the wave vectors of which lie in a small solid angle in the vicinity of the direction of the incident wave. This wave packet is diffracted by the second (lower) part of the crystal. The well-known condition for the maximum of the intensity with respect to the crystal position (resulting from the diffraction theory at Born approximation) (Bohm, 1958)

$$\mathbf{K}_0 - \mathbf{K} = \mathbf{H} \qquad (1)$$

reduces then to

$$|\mathbf{K}_0||\mathbf{K}| \cos(\mathbf{K}_0,\mathbf{K}) - \mathbf{K}^2 = \mathbf{HK} . \qquad (2)$$

Here $\mathbf{K}_0$, $\mathbf{K}$, $\mathbf{H}$ are vectors of the incident and diffracted waves and of the reciprocal lattice, respectively.

It is a matter of dynamical theory to give the limits for the validity of this model. But it seems clear we can use the model for the case of a thin crystal. Here the experiment may be arranged in such a way that we produce a suitable wave packet by means of an electron lens and we allow this packet to be diffracted by a crystal (Kossel & Möllenstedt, 1942).

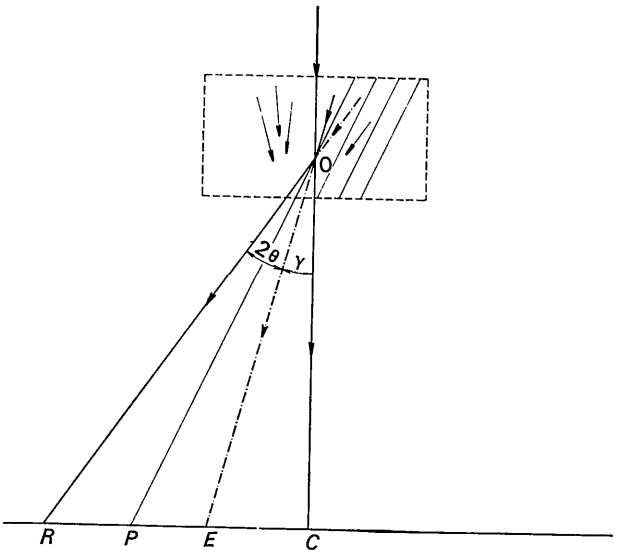

Fig. 1. Kikuchi geometrical model.

Derivation of the equation of Kikuchi lines

For practical use it is necessary to transform the equation of Kikuchi cones (2) into a suitable reference frame. We shall give the form of this equation in a Cartesian reference frame arbitrarily placed in the plane of the screen (photographic plate).

Let us denote by $\mathbf{E}_1,\mathbf{E}_2,\mathbf{E}_3$ the unit vectors of the space lattice ($\mathbf{E}_1\mathbf{E}_2=\cos\gamma$, $\mathbf{E}_2\mathbf{E}_3=\cos\alpha$, $\mathbf{E}_3\mathbf{E}_1=\cos\beta$) and by $\mathbf{S}$ the vector $(|\mathbf{S}|/|\mathbf{K}|)\mathbf{K}=x\mathbf{E}_1+y\mathbf{E}_2+z\mathbf{E}_3$. Then, using the relations $|\mathbf{H}|=4\pi\sin\theta/\lambda=2\pi/d_{hkl}$, where $\theta=(1/2)(\mathbf{K}_0,\mathbf{K})$ is the Bragg angle, $\lambda=2\pi/|\mathbf{K}_0|$ is the wave length of both primary and reflected electrons and d_{hkl} is the spacing of the (hkl) plane, and putting $\omega=h(d_{hkl}/a)$, $\mu=k(d_{hkl}/b)$, $\nu=l(d_{hkl}/c)$, we obtain the equation of Kikuchi cones in the crystallographic reference frame (with unit basic vectors)

$$S^+MS=0 \tag{3a}$$

where

$$S=\begin{pmatrix}x\\y\\z\end{pmatrix}\quad M=\begin{pmatrix}\omega^2 & \omega\mu & \omega\nu\\ \omega\mu & \mu^2 & \mu\nu\\ \omega\nu & \mu\nu & \nu^2\end{pmatrix}-\sin^2\theta\begin{pmatrix}1 & \cos\gamma & \cos\beta\\ \cos\gamma & 1 & \cos\alpha\\ \cos\beta & \cos\alpha & 1\end{pmatrix}. \tag{3b}$$

Now we choose the following transformations to obtain a suitable orthogonal reference frame. (1) We turn $\mathbf{E}_1,\mathbf{E}_2,\mathbf{E}_3$ to the position $\mathbf{E}_1',\mathbf{E}_2',\mathbf{E}_3'$ in the plane $(\mathbf{E}_1,\mathbf{E}_3)$, $(\mathbf{E}_1',\mathbf{E}_2)$, $(\mathbf{E}_2',\mathbf{E}_3)$ respectively, so that $\mathbf{E}_1'\mathbf{E}_2'=\mathbf{E}_1'\mathbf{E}_3'=\mathbf{E}_2'\mathbf{E}_3'=0$. The transformation matrices are denoted by $T_\beta,T_\gamma,T_\alpha$. (2) We turn the reference frame around $\mathbf{E}_2',\mathbf{E}_1'',\mathbf{E}_3'''$ by an angle φ,ψ,χ so that $\mathbf{E}_1'',\mathbf{E}_2''$ will be parallel to the screen and $\mathbf{E}_1''',\mathbf{E}_2'''$ will lie in a choosen direction, respectively. The transformation matrices are denoted by T_φ,T_ψ,T_χ.

The equation of the Kikuchi cone is then (in the Cartesian reference frame, two axes of which are parallel to the screen and one of them has a chosen direction)

$$S^+TMT^+S=0\,, \tag{4a}$$

where

$$T=T_\chi T_\psi T_\varphi T_\alpha T_\gamma T_\beta\,. \tag{4b}$$

The equation of the lattice plane is

$$(\omega\mu\nu)T^+S=0\,. \tag{5}$$

The equation of Kikuchi lines or the equation of the line of intersection of the lattice plane with the screen is obtained substituing $z=L$ in equations (4) and (5), L being the specimen to plate distance.

The form of the transformation matrices is simple, for they describe a simple geometrical operation;

$$T_\beta=\begin{pmatrix}\sec\beta & 0 & -\operatorname{ctg}\beta\\ 0 & 1 & 0\\ 0 & 0 & 1\end{pmatrix},\quad T_\gamma=\begin{pmatrix}1 & 0 & 0\\ -\operatorname{ctg}\gamma' & \sec\gamma' & 0\\ 0 & 0 & 1\end{pmatrix},$$

$$T_\alpha=\begin{pmatrix}1 & 0 & 0\\ 0 & 1 & 0\\ 0 & -\operatorname{ctg}\alpha' & \sec\alpha'\end{pmatrix}, \tag{6a}$$

where

$$\gamma'=\cos^{-1}[(\cos\gamma-\cos\beta\cos\alpha)/\sin\beta]\,,$$
$$\alpha'=\cos^{-1}[\cos\alpha/\sin\gamma']\,; \tag{6b}$$

$$T_\varphi=\begin{pmatrix}\cos\varphi & 0 & \sin\varphi\\ 0 & 1 & 0\\ -\sin\varphi & 0 & \cos\varphi\end{pmatrix},\quad T_\psi=\begin{pmatrix}1 & 0 & 0\\ 0 & \cos\psi & -\sin\psi\\ 0 & \sin\psi & \cos\psi\end{pmatrix},$$

$$T_\chi=\begin{pmatrix}\cos\chi & -\sin\chi & 0\\ \sin\chi & \cos\chi & 0\\ 0 & 0 & 1\end{pmatrix}. \tag{6c}$$

Practical use of the equation of Kikuchi lines

The equation of Kikuchi lines involves the following parameters: characteristics of the crystal position, that is the specimen to plate distance L and three angles φ,ψ,χ; lattice characteristics, that is the lattice parameters a,b,c and the angles of the crystallographic axes α,β,γ; the coordinates of vector $\mathbf{H}$ h,k,l; the electron wave length λ.

In practice the pattern measurement is not of high accuracy in many cases and the well-known more approximative expressions are adequate. Our formulae can then be used for estimations of the accuracy of these approximative expressions.

Measurements taken from good P-patterns have an accuracy exceeding that obtained by other methods. We illustrate it by two examples here.

(i) Measurement of the angle β of monoclinic lattices. We choose the position of the specimen so that $\varphi=\psi=\chi=0$ and the lines due to the planes $(h_ik_il_i)$ and $(h_jk_jl_j)$, for which $h_i=h_j$. Using equation (5) we obtain for the angle β

$$\beta=\operatorname{tg}^{-1}[x_0/(ny_0+L)],\ n=(c/b)(k_i-k_j)/(l_i-l_j)\,. \tag{7}$$

Here $[x_0,y_0]$ are the coordinates of the point of intersection of the $(h_ik_il_i)$ with the $(h_jk_jl_j)$ lines of intersection with the plate, measured on the plate. Considering the accuracy of the measurements of x_0, y_0 to be about 1×10^{-2}, one can see that the accuracy of the determination of the angle β is very good.

(ii) Precise determination of the orientation of the specimen. Let us rewrite equation (5) in the form

$$a_1x+a_2y+a_3L=0\,. \tag{8}$$

Having determined the equation of the line of intersection of the (hkl) plane with the photographic plate, we obtain the values a_1,a_2,a_3, and the value a_3 is nothing else than the cosine of the angle between the perpendiculars to the lattice plane (hkl) and to the screen.

In our examples we have used equation (5) which is simpler than equation (4) of Kikuchi lines. We have supposed here the coordinate of the point on the line of intersection of the lattice plane with the plate to be the mean value of the coordinates of the corresponding points of the extinction and reflection lines. We shall give the accuracy of this approximation. Let C (Fig. 1) be the spot of the incident beam; P is a point on the

line of intersection of the lattice plane with the plate, and E and R are the corresponding points on the extinction and reflexion Kikuchi lines respectively. An elementary calculation gives

$$\delta_{\mathrm{rel}}=(RP-PE)/(RP+PE)=\mathrm{tg}\,\theta\,\mathrm{tg}(\theta+\gamma)\,. \quad (9)$$

Here θ is the Bragg angle and γ is the deviation of the diffracting beam from the direction of the incident beam.

It is useful to consider in individual cases whether it is better to use equation (5) (with the approximation given above) or equation (4) (where we need to know the wavelength). For practical details of pattern measurement see Wilman's (1948) paper.

Conclusion

Using the Kikuchi model the equation of Kikuchi lines has been derived in a quite general case, in which diffraction by the triclinic lattice in an arbitrarily chosen position takes place. Thus, we have shown the possibility of performing various crystallographic measurements with good accuracy.

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A Measurement of the Absorption Coefficients of Mn, Fe, and Ti for Ag $K\alpha$ Radiation

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The absorption coefficients of Mn, Fe and Ti have been measured to an accuracy of better than ±0·6% with monochromatic Ag $K\alpha$ radiation. The absorption coefficient for Fe is in excellent agreement with Cooper's measured value.

Cooper (1965) measured the mass absorption coefficients of Al, V, Cr, Fe, Co, Ni and Cu. Utilizing Walter's (1927) empirical equation:

$$(\mu/\varrho)\frac{A}{N}=2{\cdot}64\times10^{-26}Z^{3{\cdot}94}\lambda^3 \quad (1)$$

in which μ/ϱ = mass absorption coefficient
A = atomic weight
N = Avogadro's number
Z = atomic number
λ = wavelength

one may plot these values of $(\mu/\varrho)A$ *versus* $Z^{3{\cdot}94}$ and determine by interpolation the mass absorption coefficient of the other elements of this series. However, this method can lead to values which are only accurate to within 2% whereas precise intensity measurements require a determination of the absorption coefficient to less than 1%. This investigation is a direct determination of the mass absorption coefficients of Mn, Fe and Ti.

The experimental set-up employed a standard General Electric XRD-5 spectrogoniometer with a high intensity Ag target tube operated at 40 kV, 25 mA, a singly bent lithium fluoride monochromator and palladium filters. Scintillation counters were used to monitor the beam as well as determine I/I_0. Positional micrometers located different areas of the specimen in the beam path. The monochromator geometry was adjusted until the lattice parameter, a_0, of a silicon single crystal (using a Cohen least-squares analysis) agreed with the most precise value of a_0 available (Straumanis, Borgeaud & James, 1961).

Three Mn specimens and one each of Fe and Ti were utilized in the absorption measurements. In order to optimize the accuracy of transmission measurements the thickness of all specimens was approximately equal to $2/\mu$. The three electrolytic Mn plates,* purity 99·78%, were approximately 0·006″ thick. The first

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