Acta Cryst. (1973). A**29**, 38

Dynamical Treatment of Kikuchi Patterns

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(*Received* 15 *May* 1972; *accepted* 3 *July* 1972)

A dynamical theory of Kikuchi patterns from thick crystals is developed, which takes into account the absorption of both the elastically and inelastically scattered electrons. The wave function describing the state of an inelastically scattered electron due to an elementary excitation of core electrons of the crystal atoms is calculated. The general formulae for the intensity of the pair of Kikuchi lines (hkl) and ($\bar{h}\bar{k}\bar{l}$) and bands are obtained. The intensity profiles of Kikuchi lines and bands are analyzed. For a thick crystal the 'defect' line contrast and band contrast are reversed as a result of anomalous absorption of the inelastically scattered electrons. This is in accordance with observed experimental data.

1. Introduction

Since Kikuchi lines were discovered (Kikuchi, 1928) a number of investigations have been carried out to resolve the Kikuchi-pattern problem (Laue, 1935, 1948; Lamla, 1938; Artmann, 1949; Fues & Riedel, 1949; Kainuma, 1955; Takagi, 1958; Fujimoto & Kainuma, 1963; Okamoto, Ichinokawa & Ohtsuki, 1971; Ishida, 1970, 1971). Evidently a complete theory must contain an adequate description of sufficiently complicated phenomena such as the different physical origins of the inelastic scattering of a primary beam. It is necessary to consider the particular values of energy losses and electron angular distribution for each mechanism of inelastic scattering, the subsequent propagation of the inelastically scattered electrons in certain directions near the Bragg reflexion and the true dynamical effects: many-beam scattering, 'Pendellösung fringes', anomalous absorption *etc.*

Further, the necessary condition for the development of a complete theory is the analysis of experimental data (Shinohara & Matsukawa, 1933; Boersch, 1937; Pfister, 1953; Nakai, 1970; Watanabe, 1955; Raether, 1962; Meyer-Ehmsen, 1969; Ichinokawa, Kamigaki & Ohtsuki, 1969) which enables one to estimate the relative contributions of various physical effects to the geometry and intensity distribution of the Kikuchi patterns. The contrast reversal of Kikuchi bands observed by Shinohara & Matsukawa (1933), Boersch (1937), Pfister (1953) and Nakai (1970) is experimental evidence that dynamical effects (anomalous absorption in particular) directly influence Kikuchi patterns. From experimental data (Watanabe, 1955; Raether, 1962; Meyer-Ehmsen, 1969; Ichinokawa, Kamigaki & Ohtsuki, 1969) it follows that inelastically scattered electrons with small energy losses (approximately 0 up to 100 eV) contribute to Kikuchi-pattern formation. Kikuchi patterns are formed by inelastic scattering of the incident and diffracted electrons (waves) with a simultaneous change of the phonon, plasmon and core-electron excitation states of the crystal. Another characteristic of the processes under consideration is the creation of the wide fan of scattered particles (waves) in a crystal, which provides the large angular diffraction pattern. It seems reasonable that such a divergent beam cannot arise solely from single inelastic scattering with the energy losses mentioned above.

The theory of Kikuchi lines was first proposed by Laue (1935, 1948). He used the reciprocity theorem for the explanation of Kikuchi patterns. Laue's original theory described correctly the geometrical position of Kikuchi lines but did not explain the black-white contrast of pairs of lines or Kikuchi band formation. Owing to this, Kainuma (1955) generalized the reciprocity theorem to the case of inelastically scattered electrons and applied it to determine the intensity distribution of Kikuchi lines and bands. Kainuma's theory qualitively explained the Kikuchi patterns from a non-absorbing crystal. The theory was further developed by Takagi (1958), Fujimoto *et al.* (1963), Okamoto *et al.* (1971) and Ishida (1970, 1971).

As is shown by Takagi (1958), temperature diffuse scattering (one phonon process) gives rise to Kikuchi lines in the region of a Laue spot.

Fujimoto *et al.* (1963) and Okamoto *et al.* (1971) analysed the relative contributions of phonon and plasmon excitations, as well as the excitations of core electrons of the crystal atoms, to the Kikuchi patterns. For this, it was necessary to take into account explicitly all elementary excitations in the corresponding interaction Hamiltonian of the 'incident electron–crystal', which might cause the inelastic scattering. For the mechanisms of inelastic scattering mentioned above numerical calculations of the Kikuchi pattern contrast from a Si single crystal (reflexion 220, energy 80 keV) were carried out.

Bearing in mind the theoretical description of Kikuchi patterns one has to point out two main failures of the existing theories. Firstly, nowadays there is no theory of Kikuchi pattern formation at large angles of incidence. Evidently such Kikuchi patterns are formed by the multiple scattering of incident electrons in a crystal. Secondly, there is no dynamical theory of

Kikuchi patterns which simultaneously takes into account the coherent scattering and absorption both for the elastically and inelastically scattered electron waves. Ishida (1970, 1971, *cf.* Okamoto *et al.*, 1971) considered the absorption of electron waves inside a crystal by a method similar to the phenomenological calculation of absorption of the diffuse one-phonon scattered X-rays for the case of Laue diffraction (Afanas'ev, Kagan & Chukhovskii, 1968; Chukhovskii, 1968*a*). As shown by Chukhovskii, this method does not enable one to describe the fine interference effects of inelastically scattered particles in a crystal.

The purpose of the present paper is to give a dynamical theory of Kikuchi patterns taking into account the absorption of both elastically and inelastically scattered electrons. A set of dynamical equations is derived for elastic and inelastic electron waves, based on a generalization of the method developed by Afanas'ev *et al.* (1968) and Chukhovskii (1968*a*, *b*). The derivation is briefly presented in Section 2. Also in this section the wave function describing the state of an inelastically scattered electron due to an elementary excitation of core electrons of the crystal atoms is calculated. The general formulae for the intensity of the pair of the Kikuchi lines hkl and $\bar{h}\bar{k}\bar{l}$ and bands are obtained (Section 3). The formulae can be easily generalized for phonon and plasmon mechanisms of the inelastic scattering of electrons in a crystal. In Section 4 the intensity of Kikuchi lines and bands is analysed and special attention is paid to the treatment of the Kikuchi-pattern contrast depending on crystal thickness.

The results obtained in the paper are assumed to describe correctly the intensity distribution of the Kikuchi patterns for large angles with respect to the incident electron beam.

2. Derivation of the general formulae

The motion of an electron inside a crystal is governed by the Schrödinger equation as follows:

$$\left(-\frac{\hbar^2\Delta}{2m_e}+H_{\rm cr}+H_{\rm int}\right)\psi=E\psi\,. \tag{2.1}$$

Here $H_{\rm cr}$, $-\hbar^2\Delta/2m_e$, $H_{\rm int}$ are respectively the Hamiltonians of a crystal, the electrons which fall upon and are scattered by the crystal, and 'electron–crystal' interaction; E is the total energy of the entire system, m_e is the electron mass; $\hbar$ is Plank's constant.

The wave function of the entire system can be represented in the form

$$\psi=\sum_{\mathbf{k}\{n_s\}\{n\}} c_{\mathbf{k}\{n_s\}\{n\}}|\mathbf{k}\rangle|\{n_s\}\rangle|\{n\}\rangle\,. \tag{2.2}$$

In this expression $|\mathbf{k}\rangle$ is the plane wave function

$$|\mathbf{k}\rangle=V^{-1/2}\exp(i\mathbf{kr})\,.$$

(V is the crystal volume); $|\{n_s\}\rangle$ is the eigenfunction of the phonon system being characterized by the set of the phonon occupation numbers $\{n_s\}$; $|\{n\}\rangle$ is the eigenfunction of the electronic system with the occupation numbers of the excited electronic states inside a crystal $\{n\}$ which themselves can be divided into the excitations of the valence electrons and core electrons of crystal atoms. Notice that the multiplicative representation of the crystal eigenfunction $|\{n_s\}\rangle\ |\{n\}\rangle$ is correct when the electron–phonon interaction inside a crystal can be neglected.

The interaction Hamiltonian is made up of two parts, corresponding to the interaction of the incident electron with single individual atoms, $H^{(1)}_{\rm int}$, and valence electrons $H^{(2)}_{\rm int}$ (Chukhovskii, 1968*a*, *b*):

$$H_{\rm int}=H^{(1)}_{\rm int}+H^{(2)}_{\rm int}\,. \tag{2.3}$$

Here

$$H^{(1)}_{\rm int}=\sum_a H^{(1)}_{a\,\rm int}\,,\quad H^{(1)}_{a\,\rm int}=-\frac{4\pi e^2}{V}\sum_{\mathbf{k}}\frac{\exp(i\mathbf{kr})}{k^2}\times\left(Z_a\exp(-i\mathbf{kR}_a-i\mathbf{ku}_a)-\sum_b\exp[-i\mathbf{k}(\mathbf{R}_a+\mathbf{u}_a+\mathbf{r}_{ba})]\right) \tag{2.4}$$

$$H^{(2)}_{\rm int}=\frac{4\pi e^2}{V}\sum_{\mathbf{k}}\frac{\exp(i\mathbf{kr})}{k^2}\sum_j\exp(-i\mathbf{kr}_j) \tag{2.5}$$

where the following notations have been introduced: $\mathbf{r}$ is the position of the incident electron; $\mathbf{R}_a$ is the equilibrium position of the ath atom; $\mathbf{u}_a$ denotes the displacement due to vibrations; $\mathbf{r}_{ba}$ is the position of the bth electron inside the ath atom; $\mathbf{r}_j$ is the position of the valence electron inside a crystal; Z_a is the atomic number of the ath atom; $\mathbf{R}_a=\mathbf{R}_{\mathfrak{n}}+\mathfrak{Q}_j$, $\mathbf{R}_{\mathfrak{n}}$ is the position of $\mathfrak{n}$th elementary cell; $\mathfrak{Q}_j$ determines the position of the jth atom in the unit cell.

In accordance with (2.3) the eigenfunction of the electronic system can be represented in the form of product of the eigenfunctions corresponding to the elementary excitation of the ath atom $|v_a\rangle$ with the energy E_v and valence electronic system $|n\rangle$ with the energy E_n:

$$|\{n\}\rangle=|n\rangle\prod_a|v_a\rangle\,. \tag{2.6}$$

Now inserting (2.2) into (2.1) and utilizing (2.3)–(2.6) one finds the set of linked equations for the state amplitudes $c_{\mathbf{k}\{n_S\}\{n\}}$ (*cf. e.g.* Chukhovskii, 1968*b*):

$$(E-E_{\mathbf{k}}-E_{\{n_S\}})c_{\mathbf{k}\{n_S\}0}=(V)^{-1}\sum_{\mathbf{k}'\{n'_S\}}(H_{\rm int})^{\mathbf{k}\{n_S\}0}_{\mathbf{k}'\{n'_S\}0}c_{\mathbf{k}'\{n_S\}0}+(V)^{-1}\sum_a\sum_{\mathbf{k}'\{n'_S\}}\sum_{v\neq 0}(H^{(1)}_{a\,\rm int})^{\mathbf{k}\{n_S\}0}_{\mathbf{k}'\{n'_S\}v}c_{\mathbf{k}'\{n'_S\}av}+(V)^{-1}\sum_{\mathbf{k}'}\sum_{n\neq 0}(H^{(2)}_{\rm int})^{\mathbf{k}0}_{\mathbf{k}'n}c_{\mathbf{k}'\{n_S\}n}\,;$$

$$(E-E_{\mathbf{k}}-E_{\{n_S\}}-E_v)c_{\mathbf{k}\{n_S\}a_v}=\frac{1}{V}\sum_{\mathbf{k}'\{n'_S\}}(H^{(1)}_{a\,\rm int})^{\mathbf{k}\{n_S\}v}_{\mathbf{k}\{n'_S\}0}c_{\mathbf{k}'\{n'_S\}0}+\frac{1}{V}\sum_{b\neq a}\sum_{\mathbf{k}'\{n'_S\}}(H^{(1)}_{b\,\rm int})^{\mathbf{k}\{n_S\}0}_{\mathbf{k}'\{n'_S\}}c_{\mathbf{k}'\{n'_S\}a_v}$$

$$+\frac{1}{V}\sum_{\mathbf{k}'\{n'_S\}}\sum_{\nu\neq 0}(H^{(1)}_{a\,\mathrm{int}})^{\mathbf{k}\{n_S\}\nu}_{\mathbf{k}'\{n'_S\}\nu'}c_{\mathbf{k}'\{n'_S\}a\nu'}$$

$$+\frac{1}{V}\sum_{\mathbf{k}'n}(H^{(2)}_{\mathrm{int}})^{\mathbf{k}0}_{\mathbf{k}'n}c_{\mathbf{k}'\{n_S\}a\nu n}$$

$$+\frac{1}{V}\sum_{b\neq a}\sum_{\mathbf{k}'\{n'_S\}}\sum_{\nu'\neq 0}(H^{(1)}_{b\,\mathrm{int}})^{\mathbf{k}\{n_S\}0}_{\mathbf{k}'\{n'_S\}\nu'}c_{\mathbf{k}'\{n'_S\}a\nu b\nu'};$$

$$(E-E_{\mathbf{k}}-E_{\{n_S\}}-E_\nu-E_{\nu'})c_{\mathbf{k}\{n_S\}a\nu b\nu'}$$

$$=\frac{1}{V}\sum_{\mathbf{k}'\{n'_S\}}(H^{(1)}_{b\,\mathrm{int}})^{\mathbf{k}\{n_S\}\nu'}_{\mathbf{k}'\{n'_S\}0}c_{\mathbf{k}'\{n'_S\}a\nu}$$

$$+\frac{1}{V}\sum_{\mathbf{k}'\{n'_S\}}(H^{(1)}_{a\,\mathrm{int}})^{\mathbf{k}'\{n_S\}\nu}_{\mathbf{k}'\{n'_S\}0}c_{\mathbf{k}'\{n'_S\}b\nu'}+\ldots;$$

$$(E-E_{\mathbf{k}}-E_{\{n_S\}}-E_\nu-E_n)c_{\mathbf{k}\{n_S\}a\nu n}$$

$$=\frac{1}{V}\sum_{\mathbf{k}'\{n'_S\}}\sum_{\nu'}(H^{(1)}_{a\,\mathrm{int}})^{\mathbf{k}\{n_S\}\nu}_{\mathbf{k}'\{n'_S\}\nu'}c_{\mathbf{k}'\{n'_S\}a\nu n}$$

$$+\frac{1}{V}\sum_{\mathbf{k}'n'}(H^{(2)}_{\mathrm{int}})^{\mathbf{k}n}_{\mathbf{k}'n'}c_{\mathbf{k}'\{n_S\}a\nu n'}+\ldots. \qquad (2.7)$$

On the right hand side of these equations there are matrix elements of the 'electron–crystal' interaction Hamiltonian. The upper and lower indices of the matrix elements denote the final and initial state of the entire system.

Below, we restrict ourselves to the case of the Kikuchi pattern formation due to the single inelastic scattering of the incident electron beam on core electrons of the crystal atoms (the generalization of results for the cases of inelastic scattering due to the phonon and valence-electron excitations follows directly: *cf. e.g.* Okamoto *et al.*, 1971). Also, we shall neglect the back scattering of the inelastically scattered waves into the initial state, which actually means that the present problem can be solved by standard perturbation theory. This makes it possible to write down a separate set of dynamical equations for elastically and inelastically scattered waves. Successively omitting from equation (2.7) the scattering amplitudes with simultaneous change in the initial state of the crystal

$$c_{\mathbf{k}\{n_S\}\{n\}}\neq c_{\mathbf{k}\{n_S^0\}0}\,,\quad c_{\mathbf{k}\{n_S\}\{n\}}\neq c_{\mathbf{k}\{n_S^0\}a\nu}$$

($\{n_s^0\}$ is the initial state of the phonon system) and preserving only terms of order of H^2_{int} we obtain

$$\left(\frac{k_g^2}{\kappa^2}-1\right)c_{\mathbf{k}g\{n_S^0\}0}+\sum_{g'}v(\mathbf{k}_g,\mathbf{k}_{g'})c_{\mathbf{k}g'\{n\}0_S^0}=0\,, \qquad (2.8)$$

$$\left(\frac{k_h^2}{\kappa_\nu^2}-1\right)c_{\mathbf{k}_h\{n_S^0\}a\nu}+\sum_{h'}v(\mathbf{k}_h,\mathbf{k}_{h'})c_{\mathbf{k}_h'\{n_S^0\}a\nu}= \qquad (2.9)$$

$$=\sum_g v_{a\nu}(\mathbf{k}_h,\mathbf{k}_g)c_{\mathbf{k}g\{n_S^0\}0}\,,$$

where

$$v(\mathbf{k},\mathbf{k}')=N_0\frac{2m_e}{\kappa^2}\,[H_1(\mathbf{k},\mathbf{k}')+H_2(\mathbf{k},\mathbf{k}')$$
$$+H_3(\mathbf{k},\mathbf{k}')+H_T(\mathbf{k},\mathbf{k}')] \qquad (2.10)$$

$$v_{a\nu}(\mathbf{k},\mathbf{k}')=-\frac{8\pi m_e e^2}{V\kappa_\nu^2}\,\frac{\{\sum_{b_a}\exp[-i(\mathbf{k}-\mathbf{k}')\mathbf{r}_{b_a}]\}_0^\nu}{(\mathbf{k}-\mathbf{k}')^2}$$
$$\times\exp[-M_a(\mathbf{k}-\mathbf{k}')+i(\mathbf{k}'-\mathbf{k})\mathbf{R}_a]\,. \qquad (2.11)$$

Here $M_a(\mathbf{k}-\mathbf{k}')$ is the usual Debye–Waller factor; $\boldsymbol{\kappa}_\nu$ the wave vector of the inelastically scattered electrons in vacuum, $\kappa_\nu=[2m_e(E-E_\nu-E_{\{n_S^0\}})]^{1/2}$; $\mathbf{k}_h=\mathbf{k}+\mathbf{K}_h$, where $\mathbf{K}_h$ is the reciprocal lattice vector multiplied by 2π; $N_0=N/V$, where N is a number of the crystal unit-cells; here and below we put Plank's constant $\hbar=1$.

The complex coefficients $H(\mathbf{k},\mathbf{k}')$ in parentheses in (2.10) describe the scattering and absorbing properties of the medium. Derivation and physical significance of the coefficients $H_1(\mathbf{k},\mathbf{k}')$, $H_2(\mathbf{k},\mathbf{k}')$, $H_T(\mathbf{k},\mathbf{k}')$ are given by Chukhovskii (1968*b*). $H_3(\mathbf{k},\mathbf{k}')$ corresponds to the inelastic scattering of the incident electron with valence electron excitations and is equal to

$$H_3(\mathbf{k},\mathbf{k}')=\sum_{\mathbf{k}''}\sum_{n\neq 0}\left\{\frac{\langle 0|(H^{(2)}_{\mathrm{int}})^{\mathbf{k}''}_{\mathbf{k}'}|n\rangle\,\langle n|(H^{(2)}_{\mathrm{int}})^{\mathbf{k}''}_{\mathbf{k}'}|0\rangle}{E-E_{\{n_S^0\}}-E_n+i\delta}\right\}.$$
$$\delta\to+0 \qquad (2.12)$$

For further treatment the explicit form of the coefficients $H(\mathbf{k},\mathbf{k}')$ is not essential, since for analysis of the profiles of Kikuchi lines and bands (see below) we shall use the well known values of the dynamical coefficients (Hirsch, Howie, Nicholson, Pashley & Whelan, 1965)

$$v(\mathbf{k},\mathbf{k}')\equiv\mathrm{Re}\,v(\mathbf{k},\mathbf{k}')+i\,\mathrm{Im}\,v(\mathbf{k},\mathbf{k}')\,,$$
$$\mathrm{Re}\,v(\mathbf{k},\mathbf{k}')>\mathrm{Im}\,v(\mathbf{k},\mathbf{k}')>0\,.$$

Here it should be mentioned that the thermal term $H_T(\mathbf{k},\mathbf{k}')$ may result in an appreciable contribution of the electron–phonon scattering to an absorption of the incident electron beam (Chukhovskii, 1968*b*).

Consider a platelike crystal of thickness t. The intensity of inelastically scattered electrons emerging from the crystal surface $z=t$ along the direction $\boldsymbol{\kappa}_{\nu h}$ ($\boldsymbol{\kappa}_{\nu h}$ is the wave vector of an electron in vacuum) is given by

$$I(\boldsymbol{\kappa}_{\nu h},t)=\sum_a|\varphi_{a\boldsymbol{\kappa}_{\nu h}}(\mathbf{r},t)|^2 \qquad (2.13)$$

where $\varphi_{a\boldsymbol{\kappa}_{\nu h}}(\mathbf{r},t)$ is the wave function of an electron which suffers an inelastic collision at the ath atom inside a crystal.

Taking into account the continuity of the tangential component of the electron wave vector at the exit surface of a crystal one can easily find

$$\varphi_{a\boldsymbol{\kappa}_{\nu h}}(\mathbf{r},t)$$
$$=\sum c_{\mathbf{k}_h\{n_S^0\}a\nu}\exp[i\boldsymbol{\kappa}_{\nu h}\mathbf{r}+i(\mathbf{k}_{\nu h}-\boldsymbol{\kappa}_{\nu h})\mathbf{n}t] \qquad (2.14)$$

[$\mathbf{r}\equiv(\mathbf{x},\mathbf{n}z)$ and $z\geq t$, $\mathbf{n}$ is a unit vector normal to the crystal surface]. The angular distribution of the inelastically scattered electrons near the direction $\boldsymbol{\kappa}_{\nu h}$ is

the $I(\kappa_{vh}, t)$ being multiplied by the two-dimensional state density

$$\varrho(\kappa_{vh}) = \frac{V}{t}\frac{\mathrm{d}\kappa_{vhx}\mathrm{d}\kappa_{vhy}}{(2\pi)^2} = \frac{V}{t}\frac{\kappa_{vh}^2\cos\theta'}{(2\pi)^2}\,\mathrm{d}\Omega_{\kappa vh} \quad (2.15)$$

and summarized over all excited states of individual atoms of a crystal $v\neq 0$. As a result one finds

$$\frac{\mathrm{d}I}{\mathrm{d}\Omega_{\kappa_h}}(\kappa_h, t) = \frac{V\kappa_h^2}{(2\pi)^2 t}\sum_a\sum_{v\neq 0}|\varphi_{a\kappa vh}(\mathbf{r},t)|^2 . \quad (2.16)$$

(κ_h is the average wave vector of inelastically scattered electron.)

The expressions (2.14)–(2.16) as well as (2.8), (2.9) are initial ones for the solution of the problem of the transmission Kikuchi patterns in the Laue case.

3. Calculation of the intensity of the inelastically scattered electrons in the two-Beam approximation

Let the plane monochromatic electron (wave) with wave vector κ fall on the entrance surface of a crystal $z=0$. Let us restrict ourselves to the case when only two Bragg scattered waves with corresponding vectors $\mathbf{K}_1$ for elastic and $\mathbf{K}_1'$ for inelastic waves occur. Then, equations (2.8) and (2.9) can be reduced to two sets of two equations relating the amplitudes

$$c_{\mathbf{k}g\{n_s^0\}0}\equiv c_{\mathbf{k}g},\ c_{\mathbf{k}h\{n_s^0\}a_v}\equiv c_{\mathbf{k}_{vh}}\ (g,h=0,1)$$

$$\begin{cases}(-2\delta_0+v_0)c_{\mathbf{k}0}+v_{-1}c_{\mathbf{k}1}=0\\ v_1c_{\mathbf{k}0}+(-2\delta_1+v_0)c_{\mathbf{k}1}=0\end{cases} \quad (3.1a)$$

$$\begin{cases}(-2y_0+v_0')c_{\mathbf{k}v0}+v_{-1}'c_{\mathbf{k}v1}=v_{av0}^{(0)}c_{\mathbf{k}0}+v_{av1}^{(0)}c_{\mathbf{k}1}\\ v_1'c_{\mathbf{k}v0}+(-2y_1+v_0')c_{\mathbf{k}v1}=v_{av0}^{(1)}c_{\mathbf{k}0}+v_{av1}^{(1)}c_{\mathbf{k}}\ .\end{cases} \quad (3.1b)$$

Here the following notations have been introduced:

$$\mathbf{k}_{0,1}=\boldsymbol{\kappa}_{0,1}+\kappa_{0,1}\frac{\delta_{0,1}}{\gamma_{0,1}}\mathbf{n}\,,\quad \gamma_{0,1}=\cos(\mathbf{n},\hat{\boldsymbol{\kappa}}_{0,1})\simeq 1\,, \quad (3.2a)$$

$$v(\mathbf{k},\mathbf{k}+\mathbf{K}_1)=v_{-1}\,,\quad v(\mathbf{k}+\mathbf{K}_1,\mathbf{k})=v_1\,,$$

$$\mathbf{k}_{v0,1}=\boldsymbol{\kappa}_{v0,1}+\kappa_{v0,1}\frac{y_{0,1}}{\gamma_{0,1}}\mathbf{n}\,,\quad \gamma_{0,1}'=\cos(\mathbf{n},\hat{\boldsymbol{\kappa}}_{v0,1})\simeq 1\,, \quad (3.2b)$$

$$v(\mathbf{k}_v+\mathbf{K}_1',\mathbf{k}_v)=v_1'\,,\quad v(\mathbf{k}_v,\mathbf{k}_v+\mathbf{K}_1')=v_{-1}'\,,$$
$$v_{a_v}(\mathbf{k}_h,\mathbf{k}_g)=v_{avg}^{(h)}\,.$$

As is known from dynamical boundary diffraction treatment the amplitudes of elastically scattered waves are determined as follows:

$$c_{\mathbf{k}0}^{(1,2)}=\frac{2\delta_1^{(1,2)}-v_0}{v_1}c_{\mathbf{k}1}^{(1,2)}\,,\quad c_{\mathbf{k}0}^{(1)}+c_{\mathbf{k}0}^{(2)}=1\,,$$
$$c_{\mathbf{k}1}^{(1)}+c_{\mathbf{k}1}^{(2)}=0 \quad (3.3)$$

where 'anpassungs' $\delta_{0,1}^{(1,2)}$ are the solution of the dispersion equation corresponding to the set of equations (3.1a) and are equal to (*cf. e.g.* Hirsch *et al.*, 1965):

$$\delta_0^{(1,2)}=\tfrac{1}{4}(2v_0-\alpha\pm\sqrt{\alpha^2+4v_{-1}v_1})$$
$$\alpha=\frac{2\boldsymbol{\kappa}\mathbf{K}_1+\mathbf{K}_1^2}{\kappa^2}\,,\quad \delta_1^{(1,2)}=\delta_0^{(1,2)}+\frac{\alpha}{2}\,. \quad (3.4)$$

The amplitudes $c_{\mathbf{k}_{vh}}$ are determined from (3.1b) and directly expressed in terms of the elastic wave amplitudes

$$c_{\mathbf{k}_{vh}}=\left\{\sum_{g=0,1}\sum_{\tau=1,2}\frac{v_{avg\tau}^{(h)}(-2y_{h'}+v_0')-v_{h-h'}'v_{avg\tau}^{(h')}}{[(-2y_0+v_0')(-2y_1+v_0')-v_1'v_{-1}']}c_{\mathbf{k}g}^{(\tau)}\right\}_{(h\neq h')}. \quad (3.5)$$

Substituting (3.5) into (2.14) one easily finds the wave function $\varphi_{a\kappa_{vh}}(\mathbf{r})$ corresponding to the motion of the scattered electrons along the direction $\boldsymbol{\kappa}_{vh}$ in vacuum

$$\varphi_{a\kappa_{vh}}(\mathbf{r})=\sum_{\mathbf{n}.\mathbf{k}_{vh}}\sum_{g,\tau}c_{\mathbf{k}g}^{(\tau)}\frac{v_{avg\tau}^{(h)}(-2y_{h'}+v_0')-v_{h-h'}'v_{avg\tau}^{(h')}}{[(-2y_0+v_0')(-2y_1+v_0')-v_1'v_{-1}']}$$
$$\times\exp[i\boldsymbol{\kappa}_{vh}\mathbf{x}+i\mathbf{k}_{vh}\,.\,\mathbf{n}z]\,. \quad (3.6)$$

Now making use of the relation

$$k_{vhz}=\kappa_{vhz}+y_h\kappa_{vh}$$

one can go from summation over $\mathbf{n}\,.\,\mathbf{k}_{vh}$ to integration over y_h in (3.6). As a result we get

$$\varphi_{a\kappa_{vh}}(\mathbf{r})=\frac{\kappa_{vh}t}{2\pi}\exp[i\boldsymbol{\kappa}_{vh}(\mathbf{x}+\mathbf{n}z)]$$
$$\times\sum_{g,\tau}c_{\mathbf{k}g}^{(\tau)}\int_{-\infty}^{\infty}\mathrm{d}y_h\exp(i\kappa_{vh}zy_h)$$
$$\times\frac{v_{avg\tau}^{(h)}(-2y_{h'}+v_0')-v_{h-h'}'v_{avg\tau}^{(h')}}{4(y_h-\tilde{\delta}_h^{(1)})(y_h-\tilde{\delta}_h^{(2)})}\,. \quad (3.7)$$

To obtain (3.7) the following relations have been used

$$(-2y_0+v_0')(-2y_1+v_1')-v_{-1}'v_1'$$
$$=4(y_h-\tilde{\delta}_h^{(1)})(y_h-\tilde{\delta}_h^{(2)})$$
$$y_1=y_0+\frac{\alpha'}{2}\,,\quad \tilde{\delta}_1=\tilde{\delta}_0+\frac{\alpha'}{2}\,,\quad \alpha'=\frac{2\boldsymbol{\kappa}_v\,.\,\mathbf{K}_1'+(K_1')^2}{\kappa_{v0}^2} \quad (3.8)$$

where $\tilde{\delta}=\delta(\alpha')$ are 'anpassungs' of inelastically scattered electrons. Also the fact that the expression under integration in (3.7) as function of y_h has a sharp maximum near the points Re $\tilde{\delta}_h^{(1,2)}$ with width $\simeq$ Im $\tilde{\delta}_h^{(1,2)}>0$ permits us to expand the integration limits to infinity.

Direct calculations, taking account of the residue theorem in the plane of the complex variable y_h, give the following expressions for the wave function of the inelastically scattered electrons

$$\varphi_{a\kappa_{vh}}(\mathbf{r})=\begin{cases}0\,, & z<z_a\\ \varphi_{a\kappa_{vh}}^{(1)}(\mathbf{r})+\varphi_{a\kappa_{vh}}^{(2)}(\mathbf{r})\,, & z>z_a\end{cases} \quad (3.9)$$

$$\varphi^{(\sigma)}_{\mathbf{K}_{vh}}(\mathbf{r}) = \frac{i\kappa_{vh}t}{4(\tilde{\delta}^{(1)}_h - \tilde{\delta}^{(2)}_h)}(-1)^{\sigma}\sum_{g,\tau}\mathscr{J}^{\sigma,\tau}_{vgh}c^{\tau}_{\mathbf{k}g}$$
$$\times \exp[i\mathbf{k}^{(\sigma)}_{vh}(\mathbf{r}-\mathbf{R}_a)+i\mathbf{k}^{(\tau)}_g\mathbf{R}_a]$$
$$\mathscr{J}^{(\sigma,\tau)}_{vgh} = v^{(\sigma,\tau)}_{vgh'}v'_{h-h'} - v^{(\sigma,\tau)}_{vgh}(-2\tilde{\delta}^{(\sigma)}_{h'} + v'_0)\,,$$
$$(h\neq h')$$
$$v^{(\sigma,\tau)}_{vgh} = \frac{8\pi m_e e^2}{V\kappa^2_{vh}}\frac{\{\sum_{ba}\exp[-i(\mathbf{k}^{(\sigma)}_h-\mathbf{k}^{(\tau)}_g)\mathbf{r}_{ba}]\}^{v}_{0}}{(\mathbf{k}^{(\sigma)}_h-\mathbf{k}^{(\tau)}_g)^2}$$
$$\times\exp[-M_j(\mathbf{k}^{(\sigma)}_h-\mathbf{k}^{(\tau)}_g)]\,. \qquad (3.10)$$

It follows from (3.7) and (3.9) that the state of the inelastically scattered electrons inside a crystal is described by the superposition of two Bloch functions

$$\psi_{a\mathbf{K}_v}(\mathbf{r}) = \sum_{\sigma=1,2}\psi^{(\sigma)}_{a\mathbf{K}_v}(\mathbf{r})\,,\quad \psi^{(\sigma)}_{a\mathbf{K}_v}(\mathbf{r}) = \sum_{h=0,1}\varphi^{(\sigma)}_{a\mathbf{K}_{vh}}(\mathbf{r}) \qquad (3.11)$$

where the function $\psi^{(\sigma)}_{a\mathbf{K}_v}(\mathbf{r})$ corresponds to the excitation of the Bloch wave with the wave vector $\mathbf{k}^{(\sigma)}_v = \boldsymbol{\kappa}_v + \boldsymbol{\kappa}_v\tilde{\delta}^{(\sigma)}_0\mathbf{n}$ on the σth branch of dispersion surface ($\sigma = 1{\cdot}2$). It should be mentioned that the Bloch functions $\psi^{(\sigma)}_{a\mathbf{K}_v}(\mathbf{r})$ are equal to zero when $z<z_a$. Physically this is connected with the fact that in the case of Laue diffraction the energy flux density of the Bloch electron wave for each branch of dispersion surface propagates in the **z** direction.

Finally, making use of (3.9) and (2.16) and neglecting as usual (Kainuma, 1955) the dependence of the vector $\boldsymbol{\kappa}_{vh}$ on index v one obtains the intensity of Kikuchi pattern:

$$\frac{\mathrm{d}I}{\mathrm{d}\Omega_{\boldsymbol{\kappa}_h}}(\boldsymbol{\kappa}_h, t) = N_0\cos\theta'_B\,\frac{(m_e e^2)^2}{(\tilde{\delta}^{(1)}_h-\tilde{\delta}^{(2)}_h)(\tilde{\delta}^{(1)}_h-\tilde{\delta}^{(2)}_h)^*}$$
$$\times\sum_{g,\tau}\sum_{g'\tau'}\sum_{\sigma,\sigma'}(-1)^{\sigma+\sigma'}$$
$$\times\left[\frac{\exp[i\kappa_h(\tilde{\delta}^{(\sigma)}_h-\tilde{\delta}^{(\sigma')*}_h)t]-\exp[i\kappa_g(\delta^{(\tau)}_g-\delta^{(\tau')*}_{g'})t]}{i\kappa_h(\tilde{\delta}^{(\sigma)}_h-\tilde{\delta}^{(\sigma')*}_h-\delta^{(\tau)}_g+\delta^{(\tau')*}_{g'})}\right]$$
$$\times c^{(\tau)}_{\mathbf{k}g}c^{(\tau')*}_{\mathbf{k}g'}$$
$$\times\{v'_{h-h'}v'^{*}_{h-h'}S[(\mathbf{k}^{(\sigma)}_h-\mathbf{k}^{(\tau)}_g)\,,\ (\mathbf{k}^{(\sigma')}_{h'}-\mathbf{k}^{(\tau')}_{g'})^*]$$
$$-v'_{h-h'}(-2\tilde{\delta}^{(\sigma')}_{h'}+v'_0)^*$$
$$\times S[(\mathbf{k}^{(\sigma)}_h-\mathbf{k}^{(\tau)}_g)\,,\ (\mathbf{k}^{(\sigma')}_{h'}-\mathbf{k}^{(\tau')}_{g'})^*]$$
$$-v'^{*}_{h-h'}(-2\tilde{\delta}^{(\sigma)}_{h'}+v'_0)\,S[(\mathbf{k}^{(\sigma)}_h-\mathbf{k}^{(\tau)}_g)\,,\ (\mathbf{k}^{(\sigma')}_{h'}-\mathbf{k}^{(\tau')}_{g'})^*]$$
$$+(-2\tilde{\delta}^{(\sigma)}_{h'}+v'_0)(-2\tilde{\delta}^{(\sigma')}_{h'}+v'_0)^*$$
$$\times S[(\mathbf{k}^{(\sigma)}_h-\mathbf{k}^{(\tau)}_g)\,,\ (\mathbf{k}^{(\sigma')}_{h'}-\mathbf{k}^{(\tau')}_{g'})^*]\}. \qquad (3.12)$$

Here the crystal structure amplitudes for inelastic scattering, $S(\mathbf{q}_h, \mathbf{q}_{h'})$, are equal to

$$S(\mathbf{q}_h, \mathbf{q}_{h'}) = \sum_j \exp[-i(\mathbf{q}_h-\mathbf{q}_{h'})\boldsymbol{\varrho}_j - M_j(\mathbf{q}_h) - M_j(\mathbf{q}_{h'})]\,.$$
$$\times\frac{1}{q^2_h q^2_{h'}}\cdot\{Z_j - f_j(\mathbf{q}_h)f^*_j(\mathbf{q}_{h'})$$
$$+\Big(\sum_{b\neq b'}\exp(-i\mathbf{q}_h\mathbf{r}_{bj}+i\mathbf{q}_{h'}\mathbf{r}_{b'j})\Big\} \qquad (3.13)$$

[to be compared with an analogous expression for $S(\mathbf{q}_h, \mathbf{q}_{h'})$ in Kainuma (1955)].

The structure of intensity $\mathrm{d}I/\mathrm{d}\Omega_{\boldsymbol{\kappa}_h}(\boldsymbol{\kappa}_h, t)$ is such that every term on the right of (3.12) under summation corresponds to the inelastic scattering of the incident electron with simultaneous transition of the core electrons of the crystal atoms to all excited states. Both the initial and final states of the incident electron inside a crystal are described by Bloch functions.

Equations (3.12) and (3.13) completely solve the problem of Kikuchi patterns in the two-beam approximation, due to the inelastic scattering of the incident electron by the inner shells of the crystal atoms, by taking the absorption for both the elastically and inelastically scattered wave into account in the Laue case. The calculation of the other mechanisms of inelastic scattering such as scattering from phonons and valence electrons involves a change of $S(\mathbf{q}_h, \mathbf{q}_{h'})$ functions (see, for example Fujimoto *et al.*, 1963 and Okamoto *et al.*, 1971) but the general structure of the intensity (3.12) remains unchanged. Notice that in equation (3.12) for $\mathrm{d}I/\mathrm{d}\Omega_{\boldsymbol{\kappa}_h}(\boldsymbol{\kappa}_h, t)$ the refraction effect of the inelastically scattered electron waves on the exit surface of a crystal is directly considered.

4. Analysis of results

Let us consider the behaviour of the intensity (3.12) as a function of α', when the elastic waves do not suffer Bragg reflexion inside a crystal. Then, $|\alpha|\gg|v_0|$ and the state of the elastically scattered electron is described by a plane wave (with accuracy up to terms of the order of $|v_0/\alpha|\ll 1$). In this case the terms with $g=g'=0$ and $\tau=\tau'=1$ in (3.12) give the basic contribution to the intensity of the inelastic waves. Neglecting as usual the difference of the vectors $\mathbf{k}^{(\sigma)}_h$ and $\mathbf{k}^{(\tau)}_g$ from $\boldsymbol{\kappa}_h$ and $\boldsymbol{\kappa}_g$ when considering the functions $S(\mathbf{q}_h, \mathbf{q}_{h'})$ in (3.12), and assuming that

$$S(\mathbf{q}_h, \mathbf{q}_{h'}) = S(\mathbf{q}_{h'}, \mathbf{q}_h)$$

(which is true for centro-symmetric crystals) the intensity distribution can be brought to the form

$$\frac{\mathrm{d}I}{\mathrm{d}\Omega_{\boldsymbol{\kappa}_h}}(\boldsymbol{\kappa}_h, t) = 4\cos\theta'_B N_0(m_e e^2)^2 t\exp(-\mu_0 t)$$
$$\times\left\{\frac{\mathrm{sh}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)}{\frac{\mu_h t}{2\sqrt{1+w^2}}}\left[\mathrm{ch}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)\right.\right.$$
$$\times\left(\frac{S(\mathbf{q}_{h'},\mathbf{q}_{h'})}{2(1+w^2)}+\frac{1+2w^2}{2(1+w^2)}S(\mathbf{q}_h,\mathbf{q}_h)\right.$$
$$\left.+\frac{(-1)^h w}{1+w^2}S(\mathbf{q}_{h'},\mathbf{q}_h)\right)-\mathrm{sh}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)$$
$$\left.\times\left(\frac{S(\mathbf{q}_h,\mathbf{q}_{h'})}{\sqrt{1+w^2}}+\frac{(-1)^h w}{\sqrt{1+w^2}}S(\mathbf{q}_h,\mathbf{q}_h)\right)\right]$$

$$-\frac{\sin\left[\kappa_h t\sqrt{1+w^2}\ \mathrm{Re}(v'_{-1}v'_1)^{1/2}\right]}{\kappa_h t\sqrt{1+w^2}\ \mathrm{Re}\,(v'_{-1}v'_1)^{1/2}}$$
$$\times\left(\frac{S(\mathbf{q}_{h'},\mathbf{q}_{h'})-S(\mathbf{q}_h,\mathbf{q}_h)}{2(1+w^2)}\right.$$
$$\left.+\frac{(-1)^h w}{1+w^2}\,S(\mathbf{q}_h,\mathbf{q}_{h'})\right)\Bigg\},\quad \mathbf{q}_h=\boldsymbol{\kappa}_h-\boldsymbol{\kappa}\,. \tag{4.1}$$

In this expression the standard angle function w has been introduced

$$w=-\frac{\alpha'}{2\ \mathrm{Re}\,(v'_{-1}v'_1)^{1/2}}\simeq-\frac{\sin 2\theta'_B}{2|v'_{-1}v'_1|^{1/2}}\,\eta \tag{4.2}$$

where parameter $\eta=\theta'-\theta'_B$ is the deviation from the exact Bragg angle θ'_B; 'absorption distance' $\mu_0^{-1}=(\kappa_h\ \mathrm{Im}\ v'_0)^{-1}$ is connected with the 'normal' absorption and the anomalous absorption depends on $\mu_h=\kappa_h\ \mathrm{Im}\ v'_h$. When the electrons are scattered far from the true reflexion, *i.e.* $|w|\gg 1$, then (4.1) reduces to

$$\frac{\mathrm{d}I}{\mathrm{d}\Omega_{\boldsymbol{\kappa}_h}}(\boldsymbol{\kappa}_h,t)=4\cos\theta'_B N_0(m_e e^2)^2 t\exp(-\mu_0 t)$$
$$\times\left\{S(\mathbf{q}_h,\mathbf{q}_h)+\left[1-\frac{\sin(\kappa_h t\sqrt{1+w^2}\ \mathrm{Re}\,(v'_{-1}v'_1)^{1/2})}{\kappa_h t\sqrt{1+w^2}\ \mathrm{Re}\,(v'_{-1}v'_1)^{1/2}}\right]\right.$$
$$\times\left[\frac{S(\mathbf{q}_{h'},\mathbf{q}_{h'})-S(\mathbf{q}_h,\mathbf{q}_h)}{2(1+w^2)}\right.$$
$$\left.\left.+\frac{(-1)^h w}{1+w^2}\,S(\mathbf{q}_h,\mathbf{q}_{h'})\right]\right\} \tag{4.3}$$

and with accuracy up to a factor $\exp(-\mu_0 t)$ coincides with the corresponding expression for the Kikuchi pattern in the case of a non-absorbing crystal (Kainuma, 1955).

Now consider the situation when the electrons are scattered in a range of angles $|w|\lesssim 1$ near the true Bragg direction and, besides, the inelastically scattered waves propagate on one side of the incident spot. It is easy to see that in this case the cross-section of the inelastic scattering on the angle $(\boldsymbol{\kappa}_1,\widehat{\boldsymbol{\kappa}})$ is negligibly small compared with the crosssection on the angle $(\boldsymbol{\kappa}_0,\widehat{\boldsymbol{\kappa}})$. This means that

$$S(\mathbf{q}_1,\mathbf{q}_1)\ll S(\mathbf{q}_0,\mathbf{q}_0) \tag{4.4}$$

and pair of lines is observed on the photographic plate: the 'defect' line $\mathrm{d}I/\mathrm{d}\Omega_{\boldsymbol{\kappa}_0}(\boldsymbol{\kappa}_0,t)$ and the 'excess' line $\mathrm{d}I/\mathrm{d}\Omega_{\kappa 1}(\boldsymbol{\kappa}_1,t)$ whose profile in accordance with (4.1) is given by

$$\frac{\mathrm{d}I}{\mathrm{d}\Omega_{\boldsymbol{\kappa}_0}}(\boldsymbol{\kappa}_0,t)=4\cos\theta'_B N_0(m_e e^2)^2 t\exp(-\mu_0 t)S(\mathbf{q}_0,\mathbf{q}_0)$$
$$\times\left\{\frac{\mathrm{sh}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)}{\mu_h t/2\sqrt{1+w^2}}\left[\left(1-\frac{1}{2(1+w^2)}\right)\right.\right.$$
$$\left.\times\mathrm{ch}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)-\frac{w}{\sqrt{1+w^2}}\,\mathrm{sh}\,\frac{\mu_h t}{2\sqrt{1+w^2}}\right)\Bigg]$$
$$\left.+\frac{1}{2(1+w^2)}\,\frac{\sin(\kappa_0 t\sqrt{1+w^2}\ \mathrm{Re}\,(v'_{-1}v'_1)^{1/2})}{\kappa_0 t\sqrt{1+w^2}\ \mathrm{Re}\,(v'_{-1}v'_1)^{1/2}}\right\}, \tag{4.5}$$

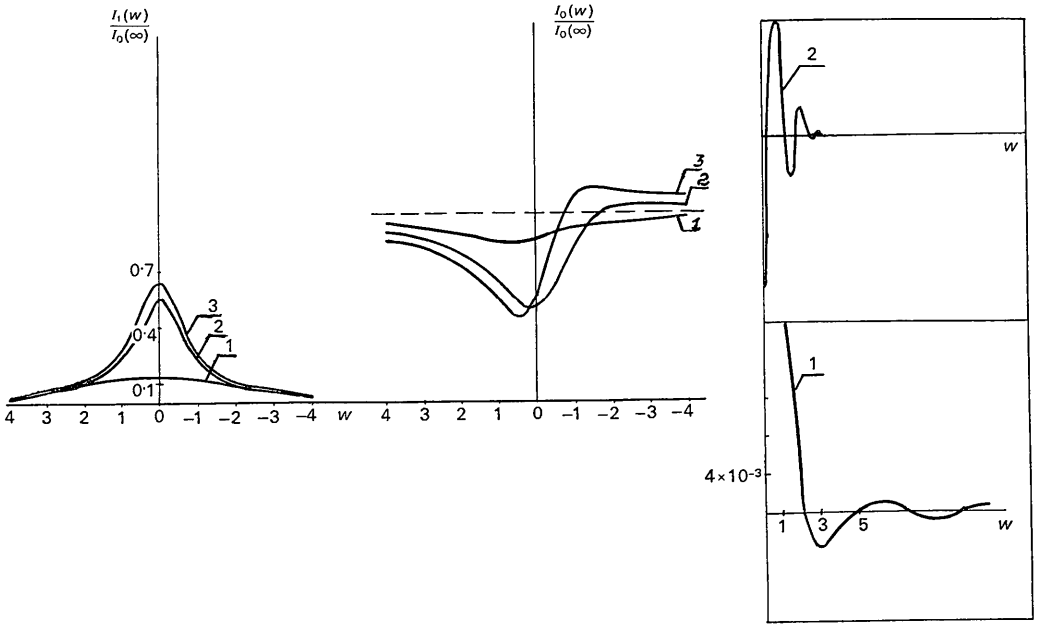

Fig. 1. Calculated profiles of Kikuchi lines for Si 440. The curves 1,2,3 refer to thicknesses of 400, 1800 and 3200 Å. The oscillating term is presented separately. The accelerating voltage is 80 kV.

$$\frac{dI}{d\Omega_{\kappa 1}}(\boldsymbol{\kappa}_1, t)=4\cos\theta'_B N_0(m_e e^2)^2 t\exp(-\mu_0 t)\,S(\mathbf{q}_0,\mathbf{q}_0)$$
$$\times\left\{\frac{\left(\mathrm{sh}\,\frac{\mu_h t}{2\sqrt{1+w^2}}\right)}{\mu_h t/2\sqrt{1+w^2}}\cdot\frac{\mathrm{ch}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)}{2(1+w^2)}\right.$$
$$\left.-\frac{1}{2(1+w^2)}\,\frac{\sin(\kappa_1 t\sqrt{1+w^2}\,\mathrm{Re}\,(v'_{-1}v'_1)^{1/2})}{\kappa_1 t\sqrt{1+w^2}\,\mathrm{Re}\,(v'_{-1}v'_1)^{1/2}}\right\}. \tag{4.6}$$

If the incident spot falls near the middle of inelastically scattered (hkl) and $(\bar{h}\bar{k}\bar{l})$ waves we have

$$S(\mathbf{q}_0,\mathbf{q}_0)=S(\mathbf{q}_1,\mathbf{q}_1)\,. \tag{4.7}$$

Then, the Kikuchi band is observed on the photographic plate. Using (4.1) and (4.7), its profile can be expressed in the form

$$\frac{dI}{d\Omega_{\kappa h}}(\boldsymbol{\kappa}_h, t)=4\cos\theta'_B N_0(m_e\,.\,e^2)^2 t\exp(-\mu_0 t)$$
$$\times\left\{\frac{\mathrm{sh}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)}{\mu_h t/2\sqrt{1+w^2}}\left[\mathrm{ch}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)\right.\right.$$
$$\times\left(S(\mathbf{q}_h,\mathbf{q}_h)+(-1)^h\frac{w}{1+w^2}S(\mathbf{q}_h,\mathbf{q}_{h'})\right)$$
$$-\mathrm{sh}\left(\frac{\mu_h t}{2\sqrt{1+w^2}}\right)\left(\frac{S(\mathbf{q}_h,\mathbf{q}_{h'})}{\sqrt{1+w^2}}\right.$$
$$\left.\left.-\frac{(-1)^h w}{\sqrt{1+w^2}}S(\mathbf{q}_h,\mathbf{q}_h)\right)\right]$$
$$-(-1)^h\frac{\sin(\kappa_h t\sqrt{1+w^2}\,\mathrm{Re}\,(v'_{-1}v'_2)^{1/2})}{\kappa_h t\sqrt{1+w^2}\,\mathrm{Re}\,(v'_{-1}v'_1)^{1/2}}$$
$$\left.\times\frac{w}{1+w^2}S(\mathbf{q}_h,\mathbf{q}_{h'})\right\}. \tag{4.8}$$

In the dynamical theory of Kikuchi patterns the formulae (4.5), (4.6) and (4.8) are basic for an analysis of the contrast of lines and bands. It should be said that recently Okamoto *et al.*, 1971; Ishida, 1970, 1971) in the case of the absorbing crystal the expressions for the profiles of lines and bands have been obtained by the solution of a phenomenological differential equation for the intensities of inelastic waves along the crystal thickness. However, as is pointed out by Chukhovskii (1968*a*), the phenomenological method mentioned above does not permit one to consider explicitly the interference of inelastic waves in corresponding expressions for intensity (the oscillating term). On the other hand the method of solution of the problem given in the present paper makes it possible to generalize the results obtained by Kainuma (1955) for the case of a thick absorbing crystal within the framework of consistent dynamical theory.

In Fig. 1 the line profiles are given for various thicknesses t for the 440 reflexion of the Si single crystal. It is interesting that in the case of the thick crystal the

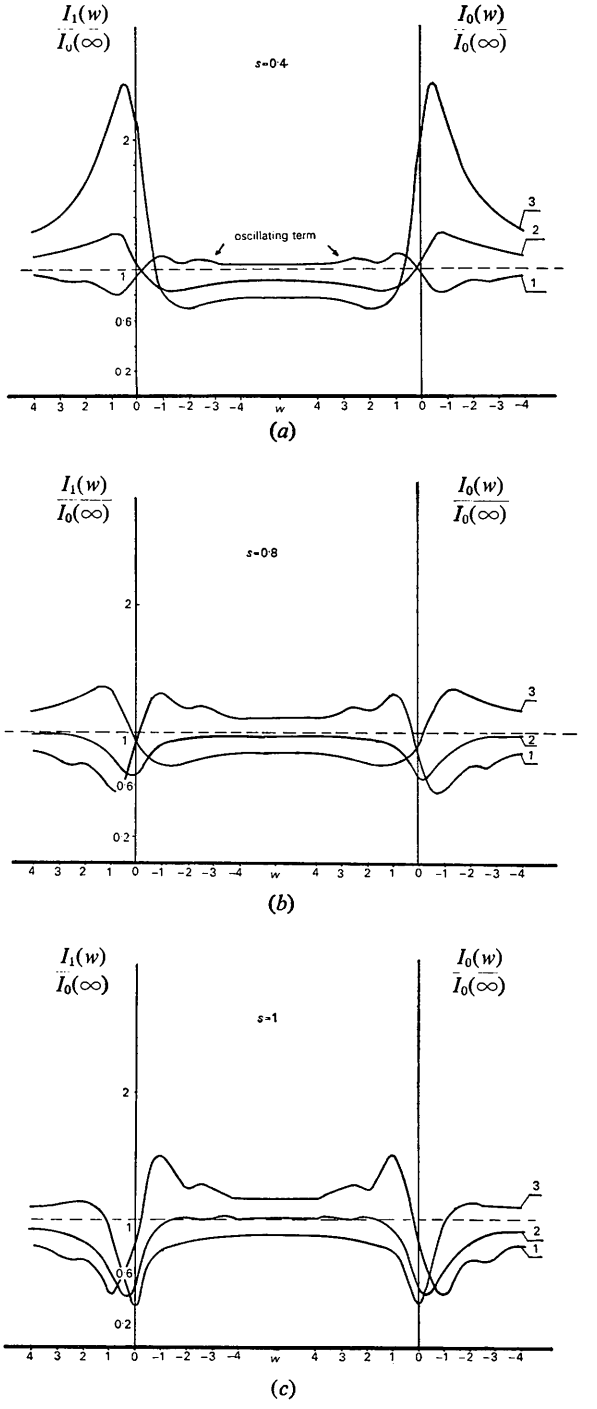

Fig. 2. Calculated profiles of the Kikuchi band of Si 220 for various values of $s=S(\mathbf{q}_0,\mathbf{q}_1)/S(\mathbf{q}_0,\mathbf{q}_0)$ equal to (*a*) 0·4, (*b*) 0·8 and (*c*) 1. The curves 1,2,3 refer to thicknesses of 400, 1800 and 3200 Å. Accelerating voltage is 80 kV. Suitable values for absorption coefficients μ_h and extinction distance $\xi_h=2\pi/\kappa\mathrm{Re}(v'_{-1}v'_1)^{1/2}$ are taken from Hirsch *et al.* (1965).

profile of the 'defect' line becomes asymmetric and the 'defect' line turns into the 'excess-deficient' line as a result of anomalous absorption. The subsidiary maxima of Kikuchi lines, corresponding to the oscillation term in (4.5) are presented separately.

Calculated profiles of the Kikuchi band for reflexion 220 of a single Si crystal are plotted in Fig. 2. From these profiles it is clear that for an absorbing crystal, the band contrast is reversed at different thicknesses depending on the parameter $s=S(\mathbf{q}_0, \mathbf{q}_1)/S(\mathbf{q}_0, \mathbf{q}_0)$. Particularly for the thick crystal this is in accordance with the results of Okamoto *et al.* (1971) and Ishida (1971) and qualitatively explains the Kikuchi patterns observed by Shinohara *et al.* (1933), Boersch (1937), Pfister (1953) and Nakai (1970). Also, for a slightly absorbing crystal, when $\mu_h t \lesssim 1$ the band profile oscillates and the number (the amplitude) of oscillations varies directly (inversely) with the argument of w.

Conclusion

1. A consistent dynamical theory of Kikuchi patterns in two-beam approximation has been developed, which takes into account the absorption of both the elastically and inelastically scattered electrons in a crystal.
2. The formulae for calculation of the intensity profiles have been obtained.
3. The theory qualitatively explains the change of the Kikuchi patterns with increase in the crystal thickness.
4. As a result of anomalous absorption of inelastically scattered waves the 'defect' line becomes 'excess-deficient' in a thick crystal.
5. The oscillating term in the intensity distribution permits one to explain the fine structure of a Kikuchi pattern.
6. The method suggested in the present paper can be applied to the many-beam diffraction of inelastically scattered electrons in thick absorbing crystals.

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Debye Temperatures of KCl, KBr and RbCl by X-ray diffraction

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(*Received* 10 *April* 1972; *accepted* 24 *July* 1972)

Debye temperatures of KCl, KBr and RbCl have been determined by X-ray diffraction from room temperature up to about 800°K using methods due to Paskin [*Acta Cryst.* (1957). **10**, 667-669] and Chipman [*J. Appl. Phys.* (1960). **31**, 2012]. The anharmonic contribution to the Debye Θ is shown to come essentially from thermal expansion. The plot of the reduced thermal expansion $\alpha/\alpha_{m/2}$ *versus* $T/Aa^2\theta^2$ gives a common curve for all the three halides. Here, $\alpha_{m/2}$ is the value of α at $T=\frac{1}{2}T_m$, T_m being the melting point, A is the mean atomic weight and a the lattice constant. An equation relating α, T and θ for the alkali halides is established for the first time. The values of the root mean square amplitudes, $(\overline{u^2})^{1/2}$, are calculated for the alkali halides from the equation and are compared with those of other workers.

Introduction

The temperature variations of the X-ray Debye temperatures of KCl and KBr have been investigated principally by Jaylakshmi & Viswamitra (KCl, 1970) and Baldwin, Pearman & Tompson (KBr, 1965). Reliable investigations on RbCl are not found in the literature.