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The Theory of Kikuchi Patterns*

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Laue's original theory (1935) of Kikuchi patterns cannot explain the fact that whether the lines appear black or white depends upon the direction of the incident beam. Although he proposed a revised theory (1948), Laue did not obtain any conclusion which could be compared with experiment. The present author has developed Laue's revised theory and discusses such conclusions.

1. Introduction

Kikuchi lines were first discovered by Kikuchi (1928) and were explained by him as follows: When a beam of electrons passes through a crystal, a divergent secondary wave may be produced in its course by some kind of scattering. As in the experiment of Rutherford & Andrade (1914), he considered the portion of each scattered wavelet which propagates in one of the directions satisfying the Bragg condition of a net plane; the reflexion by this net plane results in paired black and white lines. Kikuchi had to assume that the amplitude of the scattered wavelet is larger as the scattering angle is smaller. He also assumed, although he did not state it explicitly, that the scattered wavelet is a superposition of plane waves which have no phase relation to each other. Although he did not make the nature of the scattered wavelet clear, his assumptions were sufficient to explain the geometrical positions of the lines and their signs of intensity, i.e. black (excess) or white (defect). It is clear, however, that his assumptions could not explain the details of the intensity distribution. Moreover, Kikuchi bands and envelopes which were revealed in succeeding experiments were left unexplained.

Shinohara (1932*a*, *b*) combined the dynamical theory of diffraction with Kikuchi's assumption that the divergent wave is a superposition of plane waves, and tried to explain the bands and envelopes. Although he succeeded in part in explaining the envelopes, he failed to explain the bands because the calculated intensity was much smaller than that observed.

On the other hand, Hayashi (1934) treated kinematically the reflection by the net planes of a spherical wave emerging from an atom in the crystal. His theory was developed with the purpose of predicting the diffraction of K photoelectrons. The amplitude of the spherical wave depends upon the direction of propagation. His theory, when slightly modified, explained both Kikuchi lines and bands in a qualitative manner.

Laue (1935) proposed a theory of the Kossel patterns which are produced when X-rays emitted by an atom in a crystal are diffracted by the same crystal. He treated the diffraction of the spherical wave by the dynamical theory, skilfully avoiding mathematical difficulties by the use of the reciprocity theorem in optics. He proved the reciprocity theorem for electron waves and tried to explain Kikuchi patterns by extending Schrödinger's equation to the case where a source of electrons is present in the interior of the crystal, using the equation

$$\left\{-\frac{\hbar^2}{2m}\Delta+V(\mathbf{r})-W\right\}\varphi(\mathbf{r})=\varrho(\mathbf{r})\,, \tag{1}$$

where $\varrho(\mathbf{r})$ is different from zero only in the source and $V(\mathbf{r})$ is the potential energy of the electron in the crystal. The problem is to obtain the asymptotic solution of (1) at a point A far from the crystal, when the source is present at a point B in the crystal. Laue incorrectly assumed, perhaps for simplicity, that the source is smaller than the wave-length of electrons. His reciprocity theorem states that the solution $\varphi(\mathbf{r}_A)$ of (1) at A is given by

$$\varphi(\mathbf{r}_A)=\bar{\varphi}(\mathbf{r}_B)\,; \tag{2}$$

here $\bar{\varphi}(\mathbf{r}_B)$ is the solution at point B of

$$\left\{-\frac{\hbar^2}{2m}\Delta+V(\mathbf{r})-W\right\}\bar{\varphi}(\mathbf{r})=\bar{\varrho}(\mathbf{r})\,, \tag{3}$$

where $\bar{\varrho}(\mathbf{r})$ expresses the same source situated at point A. Since A is very far from the crystal, the wave $\bar{\varphi}(\mathbf{r})$ emitted from A can be assumed to be a plane wave when it falls on the crystal. Then $\bar{\varphi}(\mathbf{r}_B)$ can be calculated by using the ordinary dynamical theory of diffraction. Hereafter we shall call $\bar{\varphi}(\mathbf{r})$ the *reciprocal wave*.

Laue's theory is superior to former theories in that it treats the spherical wave and adopts the dynamical theory. His theory was extended by Lamla (1938*a*, *b*), Artmann (1947*a*, *b*, 1948*a*, *b*, 1949) and Fues & Riedel

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(1949) for the explanation of Kikuchi envelopes and bands.

However, there is a defect which cannot be overlooked. According to Laue's theory, the intensity of the pattern is perfectly determined by the orientation of the crystal relative to the photographic plate, independently of the direction of the primary beam. Actually, observed intensity depends upon the direction as follows: of the pair of lines, the line which lies nearer the incident spot is always white, while the other is always black; therefore a line which first lies nearer the incident spot and is white changes to black when the crystal is rotated and the line carried farther away from the incident spot (Fig. 1).

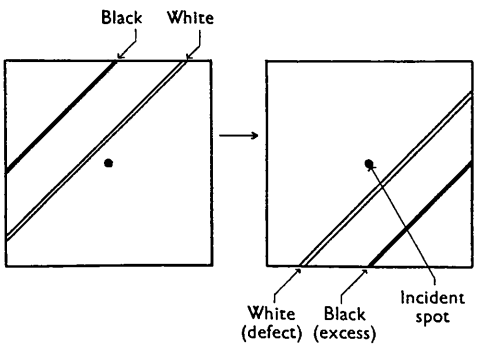

Fig. 1.

As suggested by Uyeda (1936), Fues (1939), and Thomson & Cochrane (1939), the cause of the defect of the theory lies in the assumption that the amplitude of the spherical wave near the source does not depend upon the direction of propagation, which is true only if the source is very small.

Thereafter, Laue (1948) presented his theory in revised form, in which the function $\varrho(\mathbf{r})$ in (1) is given as the result of a theoretical treatment of inelastic scattering. In this revised theory, $\varrho(\mathbf{r})$ is a function extending over the crystal. He generalized the reciprocity theorem, which was formerly applicable only to point sources, to the case where $\varrho(\mathbf{r})$ has finite extension. But he did not further develop the theory.

Independently of Laue's work, the present author developed the same theory and thereby eliminated the defect of Laue's original theory. The purpose of the present paper is to give a comprehensive description of the author's theory.

2. General treatment of inelastic scattering of an electron*

(*A*) *Differential equation for scattered waves*

In this section we apply the ordinary perturbation method of stationary states to the scattering of an electron by a scatterer composed of many atoms. The wave equation for the entire system may be written

$$\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+H(\mathbf{q})+V(\mathbf{r},\mathbf{q})-E\right\}u(\mathbf{r},\mathbf{q})=0\,, \qquad (4)$$

where $\mathbf{r}$ is the coordinate of the electron which falls upon, and is scattered by, the scatterer and $\mathbf{q}$ is the abbreviation of $\mathbf{q}_1, \sigma_1, \mathbf{q}_2, \sigma_2, \ldots, \mathbf{q}_t, \sigma_t, \ldots, \mathbf{q}_z, \sigma_z$, which are the space and spin coordinates of the other electrons in the scatterer.

The eigenfunctions for the scatterer satisfy

$$H(\mathbf{q})\Psi_0(\mathbf{q}) = E_0\Psi_0(\mathbf{q})\,,$$

and

$$H(\mathbf{q})\Psi_i(\mathbf{q}) = E_i\Psi_i(\mathbf{q})\,, \qquad (5)$$

where the suffixes 0 and i refer respectively to the ground state and excited states. The wave function of the entire system $u(\mathbf{r},\mathbf{q})$ can be expanded in the form

$$u(\mathbf{r},\mathbf{q}) = \varphi_0(\mathbf{r})\Psi_0(\mathbf{q})+\left(\sum_{i\neq 0}+\int\right)\varphi_i(\mathbf{r})\Psi_i(\mathbf{q})\,, \qquad (6)$$

where $\varphi_0(\mathbf{r})$ is the wave function of both the incident and the elastically scattered electron and $\varphi_i(\mathbf{r})$'s are the wave functions of the inelastically scattered electron related to the ith excited state of the scatterer. We assume in the following that $\left(\sum_{i\neq 0}+\int\right)\varphi_i(\mathbf{r})\Psi_i(\mathbf{q})$ is small compared with $\varphi_0(\mathbf{r})\Psi_0(\mathbf{q})$. Let us put

$$\Omega(\mathbf{r},\mathbf{q}) = V(\mathbf{r},\mathbf{q})-V_{00}(\mathbf{r})\,, \qquad (7)$$

where the matrix element V_{00} is defined by†

$$V_{00}(\mathbf{r}) = \int \Psi_0^*(\mathbf{q})V(\mathbf{r},\mathbf{q})\Psi_0(\mathbf{q})d\mathbf{q}\,; \qquad (8)$$

let us further assume $\Omega(\mathbf{r},\mathbf{q})$ to be small compared with V_{00}.

Substituting (6) and (7) in (4), we obtain the following relations for the zero- and first-order quantities:

$$\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+H(\mathbf{q})+V_{00}(\mathbf{r})-E\right\}\varphi_0(\mathbf{r})\Psi_0(\mathbf{q}) = 0\,, \qquad (9)$$

$$\left\{-\frac{\hbar^2}{2m}\Delta_{\mathbf{r}}+H(\mathbf{q})+V_{00}(\mathbf{r})-E\right\}\left(\sum_{i\neq 0}+\int\right)\varphi_i(\mathbf{r})\Psi_i(\mathbf{q}) +\Omega(\mathbf{r},\mathbf{q})\varphi_0(\mathbf{r})\Psi_0(\mathbf{q}) = 0\,. \qquad (10)$$

By multiplying (9) and (10) respectively by $\Psi_0^*(\mathbf{q})$ and $\Psi_i^*(\mathbf{q})$, and integrating with respect to $\mathbf{q}$, we obtain

$$\left\{-\frac{\hbar^2}{2m}\Delta+V_{00}(\mathbf{r})-W_0\right\}\varphi_0(\mathbf{r}) = 0\,, \qquad (11)$$

and

$$\left\{-\frac{\hbar^2}{2m}\Delta+V_{00}(\mathbf{r})-W_i\right\}\varphi_i(\mathbf{r}) = -V_{i0}(\mathbf{r})\varphi_0(\mathbf{r})\,, \qquad (12)$$

where

* This section is essentially the same as Laue's revised theory, but it is given here as the author developed the theory. This section may be useful for an understanding of the following sections.

† In this paper the asterisk on $\Psi_0^*(\mathbf{q})$, etc. denotes the complex conjugate.

$$W_0 = E - E_0 , \tag{13}$$

$$W_i = E - E_i , \tag{14}$$

and

$$V_{i0}(\mathbf{r}) = \int \Psi_i^*(\mathbf{q}) \Omega(\mathbf{r}, \mathbf{q}) \Psi_0(\mathbf{q}) d\mathbf{q} = \int \Psi_i^*(\mathbf{q}) V(\mathbf{r}, \mathbf{q}) \Psi_0(\mathbf{q}) d\mathbf{q} . \tag{15}$$

Equation (12) corresponds to Laue's equation (1).

(B) The asymptotic solution of equation (12); *a generalization of the reciprocity theorem*

The wave function $\varphi_i(\mathbf{r})$ has the asymptotic form

$$\varphi_i(\mathbf{r}) \sim f_i(\theta, \phi) \exp(-2\pi i k_i r)/r , \tag{16}$$

where

$$k_i^2 = 2mW_i/\hbar^2 . \tag{17}$$

Let us consider here the reciprocal wave $\bar{\varphi}_i(\mathbf{r})$ which satisfies the equation

$$\left\{-\frac{\hbar^2}{2m}\Delta + V_{00}(\mathbf{r}) - W_i\right\} \bar{\varphi}_i(\mathbf{r}) = -\delta(\mathbf{r}-\mathbf{r}_A) , \tag{18}$$

where $\delta(\mathbf{r}-\mathbf{r}_A)$ is a delta function. Its asymptotic form is given by

$$\bar{\varphi}_i(\mathbf{r}) \sim \bar{f}_i(\theta, \phi) \exp(-2\pi i k_i r)/r . \tag{19}$$

Multiplying (12) by $\bar{\varphi}_i(\mathbf{r})$, (18) by $\varphi_i(\mathbf{r})$, subtracting, and integrating with respect to r, we have

$$-\frac{\hbar^2}{2m}\int \left\{\bar{\varphi}_i \Delta\varphi_i - \varphi_i \Delta\bar{\varphi}_i\right\} d\mathbf{r} = \int \varphi_i(\mathbf{r}) \delta(\mathbf{r}-\mathbf{r}_A) d\mathbf{r} - \int \bar{\varphi}_i(\mathbf{r}) V_{i0}(\mathbf{r}) \varphi_0(\mathbf{r}) d\mathbf{r} . \tag{20}$$

By the use of Green's theorem, the left-hand side vanishes, as shown in Laue's theory. Thus we obtain

$$\varphi_i(\mathbf{r}_A) = \int \bar{\varphi}_i(\mathbf{r}) V_{i0}(\mathbf{r}) \varphi_0(\mathbf{r}) d\mathbf{r} . \tag{21}$$

This result may be regarded as a generalization of the reciprocity theorem.†

3. Inelastic scattering of an electron by a crystal

(A) General formulation according to the dynamical theory of electron diffraction

According to Lamla (1938*a*), the incident and elastically scattered wave $\varphi_0(\mathbf{r})$ and the reciprocal waves $\bar{\varphi}_i(\mathbf{r})$ in the crystal are given respectively by

$$\varphi_0(\mathbf{r}) = \sum_{\mathbf{h}} \sum_{\nu} \Phi_{\mathbf{h}}^{\nu} \exp(-2\pi i \mathbf{k}_{\mathbf{h}}^{\nu} . \mathbf{r}) , \tag{22}$$

and

$$\bar{\varphi}_i(\mathbf{r}) = \sum_{\bar{\mathbf{h}}} \sum_{\bar{\nu}} \bar{\Phi}_{i\bar{\mathbf{h}}}^{\bar{\nu}} \exp(-2\pi i \bar{\mathbf{k}}_{i\bar{\mathbf{h}}}^{\bar{\nu}} . \mathbf{r}) , \tag{23}$$

† It is also a generalization of the method developed in the theory of atomic collision for the case of a spherically symmetric $V_{00}(\mathbf{r})$ (Mott & Massey, 1949).

where

$$\mathbf{k}_{\mathbf{h}}^{\nu} = \mathbf{k}_{\mathbf{0}}^{\nu} + \mathbf{h} , \qquad \bar{\mathbf{k}}_{i\bar{\mathbf{h}}}^{\bar{\nu}} = \bar{\mathbf{k}}_{i\mathbf{0}}^{\bar{\nu}} + \bar{\mathbf{h}} . \tag{24}$$

The quantities $\mathbf{h}$, $\bar{\mathbf{h}}$ are lattice vectors in the reciprocal lattice and $\nu, \bar{\nu}$ are the indices of the wave points.‡ Substituting (22) and (23) into (21), we obtain

$$\varphi_i(\mathbf{r}_A) = \sum_{\mathbf{h},\nu} \sum_{\bar{\mathbf{h}},\bar{\nu}} \bar{\Phi}_{i\bar{\mathbf{h}}}^{\bar{\nu}} \Phi_{\mathbf{h}}^{\nu} I_{i\mathbf{h}\bar{\mathbf{h}}}^{\nu\bar{\nu}} , \tag{25}$$

where

$$I_{i\mathbf{h}\bar{\mathbf{h}}}^{\nu\bar{\nu}} = \int \exp(-2\pi i \bar{\mathbf{k}}_{i\bar{\mathbf{h}}}^{\bar{\nu}} . \mathbf{r}) V_{i0}(\mathbf{r}) \exp(-2\pi i \mathbf{k}_{\mathbf{h}}^{\nu} . \mathbf{r}) d\mathbf{r} . \tag{26}$$

The interaction potential energy $V(\mathbf{r}, \mathbf{q})$ between the electron and crystal is given by

$$V(\mathbf{r}, \mathbf{q}) = e^2 \left\{ -\sum_{\mathbf{n}} \sum_{k} \frac{Z_k}{|\mathbf{r}-\mathbf{r}_k(\mathbf{n})|} + \sum_{l} \frac{1}{|\mathbf{r}-\mathbf{q}_l|} \right\} , \tag{27}$$

where $\mathbf{r}_k(\mathbf{n})$ denotes the position af the kth atom in the $\mathbf{n}$th unit cell of the crystal and $\mathbf{q}_l$ the position of any electron. The atomic number of the kth atom is Z_k. Using (26), (15) and (27), we have

$$I_{i\mathbf{h}\bar{\mathbf{h}}}^{\nu\bar{\nu}} = e^2 \int \Phi_i^*(\mathbf{q}) \Phi_0(\mathbf{q}) d\mathbf{q} \times \int d\mathbf{r} \exp\{-2\pi i (\mathbf{k}_{\mathbf{h}}^{\nu} + \bar{\mathbf{k}}_{i\bar{\mathbf{h}}}^{\bar{\nu}}) . \mathbf{r}\} \times \left\{ -\sum_{\mathbf{n}} \sum_{k} \frac{Z_k}{|\mathbf{r}-\mathbf{r}_k(\mathbf{n})|} + \sum_{l} \frac{1}{|\mathbf{r}-\mathbf{q}_l|} \right\} . \tag{28}$$

For further calculation we must use the approximation for k_i in (17) adopted by Morse (1932) and Heisenberg (1931), which is

$$k_i \approx k_0 \tag{29}$$

for all values of i which contribute appreciably to the total flux density of inelastically scattered waves. Then suffix i is omitted in $\bar{\mathbf{k}}_{i\bar{\mathbf{h}}}^{\bar{\nu}}$ and $\bar{\Phi}_{i\bar{\mathbf{h}}}^{\bar{\nu}}$ in all the following discussions.

Making use of the formula (Bethe, 1930; Wentzel, 1933)

$$\int d\mathbf{r} \exp(-2\pi i \mathbf{k} . \mathbf{r})/|\mathbf{r}-\mathbf{r}'| = \frac{1}{\pi} \exp(-2\pi i \mathbf{k} . \mathbf{r}')/\mathbf{k}^2 , \tag{30}$$

we have

$$I_{i\mathbf{h}\bar{\mathbf{h}}}^{\nu\bar{\nu}} = \frac{e^2}{\pi} (i|U_{\mathbf{h}\bar{\mathbf{h}}}^{\nu\bar{\nu}}|0)/(\mathbf{k}_{\mathbf{h}}^{\nu} + \bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})^2 , \tag{31}$$

where

$$(i|U_{\mathbf{h}\bar{\mathbf{h}}}^{\nu\bar{\nu}}|0) = \int \Psi_i^* U_{\mathbf{h}\bar{\mathbf{h}}}^{\nu\bar{\nu}} \Psi_0 d\mathbf{q} , \tag{32}$$

and

$$U_{\mathbf{h}\bar{\mathbf{h}}}^{\nu\bar{\nu}} = \sum_{l} \exp\{-2\pi i (\mathbf{k}_{\mathbf{h}}^{\nu} + \bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) . \mathbf{q}_l\} . \tag{33}$$

‡ In this paper the bar on $\bar{\mathbf{h}}$, etc. denotes a quantity related to the reciprocal wave.

Substituting (31) into (25), we obtain

$$\varphi_i(\mathbf{r}_A)=\frac{e^2}{\pi}\sum_{\mathbf{h},\nu}\sum_{\bar{\mathbf{h}},\bar{\nu}}\Phi^{\nu}_{\mathbf{h}}\bar{\Phi}^{\bar{\nu}}_{\bar{\mathbf{h}}}(i|U^{\nu\bar{\nu}}_{\mathbf{h}\bar{\mathbf{h}}}|0)/(\mathbf{k}^{\nu}_{\mathbf{h}}+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})^2\,. \quad (34)$$

We assume in this paper that the intensity of the Kikuchi pattern at A is given by the total flux density at A of the inelastically scattered electron waves

$$J(\mathbf{r}_A)=\frac{h}{m}(\sum_{i\neq 0}+\int)k_i|\varphi_i(\mathbf{r}_A)|^2\,. \quad (35)$$

Substituting (29) and (34) into (35), we obtain the basic formula for the Kikuchi pattern:

$$\begin{aligned}J(\mathbf{r}_A)&=\frac{hk_0}{m}(\sum_{i\neq 0}+\int)|\varphi_i(\mathbf{r}_A)|^2\\&=\frac{hk_0}{m\pi^2}\sum_{\mathbf{h},\nu}\sum_{\mathbf{g},\mu}\sum_{\bar{\mathbf{h}},\bar{\nu}}\sum_{\bar{\mathbf{g}},\bar{\mu}}C^{\nu\mu\bar{\nu}\bar{\mu}}_{\mathbf{hgh}\bar{\mathbf{g}}}\\&\times\Phi^{\nu}_{\mathbf{h}}\Phi^{\mu*}_{\mathbf{g}}\bar{\Phi}^{\bar{\nu}}_{\bar{\mathbf{h}}}\bar{\Phi}^{\bar{\mu}*}_{\bar{\mathbf{g}}}/(\mathbf{k}^{\nu}_{\mathbf{h}}+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})^2(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}})^2\,, \quad (36)\end{aligned}$$

where

$$C^{\nu\mu\bar{\nu}\bar{\mu}}_{\mathbf{hgh}\bar{\mathbf{g}}}=\{\sum_{i\neq 0}+\int\}(i|U^{\nu\bar{\nu}}_{\mathbf{h}\bar{\mathbf{h}}}|0)(i|U^{\mu\bar{\mu}}_{\mathbf{g}\bar{\mathbf{g}}}|0)^*. \quad (37)$$

It must be noted here that (36) fails where

$$\mathbf{k}^{\nu}_{\mathbf{h}}+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}}\approx 0\,, \quad (38)$$

as pointed out by Morse (1932).

Since (37) may be rewritten as

$$C^{\nu\mu\bar{\nu}\bar{\mu}}_{\mathbf{hgh}\bar{\mathbf{g}}}=(0|U^{\nu\bar{\nu}}_{\mathbf{h}\bar{\mathbf{h}}}U^{\mu\bar{\mu}*}_{\mathbf{g}\bar{\mathbf{g}}}|0)-(0|U^{\nu\bar{\nu}}_{\mathbf{h}\bar{\mathbf{h}}}|0)(0|U^{\mu\bar{\mu}*}_{\mathbf{g}\bar{\mathbf{g}}}|0)\,, \quad (39)$$

$C^{\nu\mu\bar{\nu}\bar{\mu}}_{\mathbf{hgh}\bar{\mathbf{g}}}$ is obtained only from the wave function of the ground state $\Psi_0(\mathbf{q})$, without any knowledge of the wave functions of the excited states $\Psi_i(\mathbf{q})$ (Waller, 1928; Morse, 1932; Heisenberg 1931).

(B) Application of the Hartree–Fock approximation

With the help of (33), the first term of (39) may be written

$$(0|U^{\nu\bar{\nu}}_{\mathbf{h}\bar{\mathbf{h}}}U^{\mu\bar{\mu}*}_{\mathbf{g}\bar{\mathbf{g}}}|0)=\sum_{t}+\sum_{t\neq s}\Sigma\,, \quad (40)$$

where

$$\begin{aligned}\sum_{t}&=\sum_{t}\int\Psi_0^*(\mathbf{q})\Psi_0(\mathbf{q})\\&\times\exp\{2\pi i(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}}-\mathbf{k}^{\nu}_{\mathbf{h}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\cdot\mathbf{q}_t\}d\mathbf{q}\,, \quad (41)\end{aligned}$$

and

$$\begin{aligned}\sum_{t\neq s}\Sigma&=\sum_{t\neq s}\int\Psi_0^*(\mathbf{q})\Psi_0(\mathbf{q})\\&\times\exp 2\pi i\{(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}})\cdot\mathbf{q}_s-(\mathbf{k}^{\nu}_{\mathbf{h}}+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\cdot\mathbf{q}_t\}d\mathbf{q}\,. \quad (42)\end{aligned}$$

The antisymmetrical wave function of the many-electron system

$$\Psi_0(\mathbf{q})=\Psi_0(\mathbf{q}_1,\sigma_1,\mathbf{q}_2,\sigma_2,\ldots,\mathbf{q}_t,\sigma_t,\ldots,\mathbf{q}_z,\sigma_z)$$

may be formed by setting up the determinant

$$\Psi_0(\mathbf{q})=\frac{1}{\sqrt{(Z!)}}\begin{vmatrix}\psi_1(\mathbf{q}_1,\sigma_1), & \psi_1(\mathbf{q}_2,\sigma_2), & \ldots, & \psi_1(\mathbf{q}_z,\sigma_z)\\ \psi_2(\mathbf{q}_1,\sigma_1), & \psi_2(\mathbf{q}_2,\sigma_2), & \ldots, & \psi_2(\mathbf{q}_z,\sigma_z)\\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\\ \psi_z(\mathbf{q}_1,\sigma_1), & \psi_z(\mathbf{q}_2,\sigma_2), & \ldots, & \psi_z(\mathbf{q}_z,\sigma_z)\end{vmatrix}, \quad (43)$$

where $\psi_j(\mathbf{q}_t,\sigma_t)$ is the Bloch one-electron wave function (of the tth electron in the jth state) as obtained in the Hartree–Fock approximation to the z-electron system of the crystal. The density of electrons in the crystal at X can be written

$$\varrho(\mathbf{X})=\sum_{j}\sum_{\zeta}\psi_j^*(\mathbf{X},\zeta)\psi_j(\mathbf{X},\zeta)\,, \quad (44)$$

where ζ is the spin coordinate.

By the help of (43) and (44), (41) turns out to be

$$\begin{aligned}\sum_{t}&=\int_{\text{crystal}}\varrho(\mathbf{X})\exp\{2\pi i(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}}-\mathbf{k}^{\nu}_{\mathbf{h}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\cdot\mathbf{X}\}d\mathbf{X} \quad (45)\\&=L(\mathbf{k}^{\mu*}_{\mathbf{0}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\mathbf{0}}-\mathbf{k}^{\nu}_{\mathbf{0}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\mathbf{0}})F(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}}-\mathbf{k}^{\nu}_{\mathbf{h}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\\&\times\exp\{2\pi i(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}}-\mathbf{k}^{\nu}_{\mathbf{h}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\cdot\mathbf{r}(\mathbf{0})\},\end{aligned}$$

where

$$\begin{aligned}&L(\mathbf{k}^{\mu*}_{\mathbf{0}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\mathbf{0}}-\mathbf{k}^{\nu}_{\mathbf{0}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\mathbf{0}})\\&\quad=\sum_{\mathbf{n}}\exp\{2\pi i(\mathbf{k}^{\mu*}_{\mathbf{0}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\mathbf{0}}-\mathbf{k}^{\nu}_{\mathbf{0}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\mathbf{0}})\cdot\mathbf{n}\}\,, \quad (46)\end{aligned}$$

$$\begin{aligned}&F(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}}-\mathbf{k}^{\nu}_{\mathbf{h}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\\&=\int_{\text{unit cell}}\varrho(\mathbf{X})\exp\{2\pi i(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}}-\mathbf{k}^{\nu}_{\mathbf{h}}-\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\cdot(\mathbf{X}-\mathbf{r}(\mathbf{0}))\}d\mathbf{X}; \quad (47)\end{aligned}$$

here $\mathbf{r}(\mathbf{0})$ is the position vector of the origin of the lattice, and $\mathbf{n}$ is the lattice vector $\mathbf{n}=n_1\mathbf{a}_1+n_2\mathbf{a}_2+n_3\mathbf{a}_3$, where $\mathbf{a}_1$, $\mathbf{a}_2$ and $\mathbf{a}_3$ are the lattice axes. $|L|^2$ gives the usual Laue function and F is the crystal structure amplitude for X-ray diffraction by the crystal.

Next, (42) turns out to be

$$\begin{aligned}&\sum_{t\neq s}\Sigma\\&=\sum_{j}\sum_{j'}\int\!\!\int_{\text{crystal}}\sum_{\zeta}\sum_{\zeta'}\psi_j^*(\mathbf{X},\zeta)\psi_j(\mathbf{X},\zeta)\psi_{j'}^*(\mathbf{X}',\zeta')\psi_{j'}(\mathbf{X}',\zeta')\\&\times\exp 2\pi i\{(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}})\cdot\mathbf{X}'-(\mathbf{k}^{\nu}_{\mathbf{h}}+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\cdot\mathbf{X}\}d\mathbf{X}d\mathbf{X}'\\&-\int\!\!\int_{\text{crystal}}\sum_{\zeta}\sum_{\zeta'}\Big|\sum_{j}\psi_j^*(\mathbf{X},\zeta)\psi_j(\mathbf{X}',\zeta')\Big|^2\\&\times\exp 2\pi i\{(\mathbf{k}^{\mu*}_{\mathbf{g}}+\bar{\mathbf{k}}^{\bar{\mu}*}_{\bar{\mathbf{g}}})\cdot\mathbf{X}'-(\mathbf{k}^{\nu}_{\mathbf{h}}+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})\cdot\mathbf{X}\}d\mathbf{X}d\mathbf{X}'\,. \quad (48)\end{aligned}$$

The first term in (48) is cancelled by

$$-(0|U^{\nu\bar{\nu}}_{\mathbf{h}\bar{\mathbf{h}}}|0)(0|U^{\mu\bar{\mu}*}_{\mathbf{g}\bar{\mathbf{g}}}|0)$$

in (39); therefore, only the second term is to be calculated. Separating the spin part of the Bloch function

$$\psi_j(\mathbf{X},\zeta)=\psi_{(j)}(\mathbf{X})\chi_j(\zeta)\,, \quad (49)$$

we have

$$\sum_j \psi_j^*(\mathbf{X},\zeta)\psi_j(\mathbf{X}',\zeta') = \sum_j \psi_{(j)}^*(\mathbf{X})\psi_{(j)}(\mathbf{X}')\chi_j^*(\zeta)\chi_j(\zeta') = \delta_{\zeta\zeta'}\sum_{(j)}\psi_{(j)}^*(\mathbf{X})\psi_{(j)}(\mathbf{X}'), \quad (50)\dagger$$

restricting ourselves to the case where all the spins are coupled. The suffix (j) in (49) and (50) is related to the (j)th state which is numbered without consideration of spins. Using (39), (40), (45), (48) and (50) we have

$$\begin{aligned} C^{\nu\mu\bar{\nu}\bar{\mu}}_{\mathbf{h}\mathbf{g}\bar{\mathbf{h}}\bar{\mathbf{g}}} &= L(\mathbf{k}_0^{\mu*}+\bar{\mathbf{k}}_0^{\bar{\mu}*}-\mathbf{k}_0^{\nu}-\bar{\mathbf{k}}_0^{\bar{\nu}})F(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) \\ &\times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\cdot\mathbf{r}(\mathbf{0})\} \\ &-2\iint_{\text{crystal}} d\mathbf{X}d\mathbf{X}'\Big|\sum_{(j)}\psi_{(j)}^*(\mathbf{X})\psi_{(j)}(\mathbf{X}')\Big|^2 \\ &\times \exp 2\pi i\{(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*})\cdot\mathbf{X}'-(\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\cdot\mathbf{X}\}. \end{aligned} \quad (51)$$

By using the approximation to be introduced in § 4, the rather complicated equation (51) reduces to

$$\begin{aligned} C^{\nu\mu\bar{\nu}\bar{\mu}}_{\mathbf{h}\mathbf{g}\bar{\mathbf{h}}\bar{\mathbf{g}}} &= L(\mathbf{k}_0^{\mu*}+\bar{\mathbf{k}}_0^{\bar{\mu}*}-\mathbf{k}_0^{\nu}-\bar{\mathbf{k}}_0^{\bar{\nu}})S(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) \\ &\times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\cdot\mathbf{r}(\mathbf{0})\}, \end{aligned} \quad (52)$$

where S is the factor which may be called *the crystal structure factor for Kikuchi patterns.*

Finally, by the use of (36) and (52) we obtain for the intensity of the Kikuchi pattern:

$$\begin{aligned} J(\mathbf{r}_A) &= \frac{hk_0e^4}{m\pi^2}\sum_{\mathbf{h},\nu}\sum_{\mathbf{g},\mu}\sum_{\bar{\mathbf{h}},\bar{\nu}}\sum_{\bar{\mathbf{g}},\bar{\mu}} L(\mathbf{k}_0^{\mu*}+\bar{\mathbf{k}}_0^{\bar{\mu}*}-\mathbf{k}_0^{\nu}-\bar{\mathbf{k}}_0^{\bar{\nu}}) \\ &\times S(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) \\ &\times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\cdot\mathbf{r}(\mathbf{0})\} \\ &\times \Phi_{\mathbf{h}}^{\nu}\Phi_{\mathbf{g}}^{\mu*}\bar{\Phi}_{\bar{\mathbf{h}}}^{\bar{\nu}}\bar{\Phi}_{\bar{\mathbf{g}}}^{\bar{\mu}*}/(\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})^2(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*})^2. \end{aligned} \quad (53)$$

4. Calculation of the crystal structure factor for Kikuchi patterns

(A) *The approximation of tight binding*

In this section we assume tight binding for the electrons of the crystal. For the sake of brevity we first consider a lattice containing only one atom at $\mathbf{r}_0$ in the unit cell. Then the Bloch function $\psi_{(j)}(\mathbf{X})$ may be constructed from the atomic functions $\phi_l(\mathbf{X}-\mathbf{r}_0(\mathbf{n}))$, (where $\mathbf{r}_0(\mathbf{n})$ is the vector from the origin of the coordinate to the atom in the $\mathbf{n}$th unit cell) as follows:

$$\begin{aligned} &\psi_{(j)}(\mathbf{X}) \equiv \psi_{l,\boldsymbol{\tau}}(\mathbf{X}) \\ &= (1/\sqrt{(N_1N_2N_3)})\sum_{\mathbf{n}}\phi_l(\mathbf{X}-\mathbf{r}_0(\mathbf{n}))\exp(-2\pi i\boldsymbol{\tau}\cdot\mathbf{r}_0(\mathbf{n})); \end{aligned} \quad (54)$$

here l indicates the lth energy band of the crystal (or lth level of the atom) and $\boldsymbol{\tau}$ is the wave vector of the electron in the crystal, given by

$$\boldsymbol{\tau} = \frac{p_1}{N_1}\mathbf{b}_1+\frac{p_2}{N_2}\mathbf{b}_2+\frac{p_3}{N_3}\mathbf{b}_3, \quad (55)$$

where p_1, p_2 and p_3 are integers satisfying the relations

$$0 \leqq p_1 \leqq N_1-1,\ 0 \leqq p_2 \leqq N_2-1,\ 0 \leqq p_3 \leqq N_3-1, \quad (56)$$

the crystal being assumed to have a volume of $((N_1\mathbf{a}_1\times N_2\mathbf{a}_2)\cdot N_3\mathbf{a}_3)$. The vectors $\mathbf{b}_1$, $\mathbf{b}_2$ and $\mathbf{b}_3$ are the reciprocal vectors to $(\mathbf{a}_i)$.

Using (54), we have

$$\begin{aligned} \sum_{(j)} &\equiv \sum_{(j)}\psi_{(j)}^*(\mathbf{X})\psi_{(j)}(\mathbf{X}') = \sum_l\sum_{\boldsymbol{\tau}}\psi_{l,\boldsymbol{\tau}}^*(\mathbf{X})\psi_{l,\boldsymbol{\tau}}(\mathbf{X}') \\ &= (1/N_1N_2N_3)\sum_{\mathbf{n}}\sum_{\mathbf{m}}\sum_l\phi_l^*(\mathbf{X}-\mathbf{r}_0(\mathbf{n}))\phi_l(\mathbf{X}'-\mathbf{r}_0(\mathbf{m})) \\ &\times \sum_{\boldsymbol{\tau}}\exp\{2\pi i\boldsymbol{\tau}\cdot(\mathbf{n}-\mathbf{m})\}. \end{aligned} \quad (57)$$

If all the energy bands are completely filled,

$$\sum_{\boldsymbol{\tau}}\exp\{2\pi i\boldsymbol{\tau}\cdot(\mathbf{n}-\mathbf{m})\}$$

is equal to $N_1N_2N_3$ for $\mathbf{n}=\mathbf{m}$ and is small compared with $N_1N_2N_3$ for $\mathbf{n}\neq\mathbf{m}$. Thus (57) may be approximated by

$$\sum_{(j)} \approx \sum_{\mathbf{n}}\sum_l\phi_l^*(\mathbf{X}-\mathbf{r}_0(\mathbf{n}))\phi_l(\mathbf{X}'-\mathbf{r}_0(\mathbf{n})). \quad (58)$$

Since the overlapping of $\phi_l(\mathbf{X}-\mathbf{r}_0(\mathbf{n}))$ and $\phi_k(\mathbf{X}-\mathbf{r}_0(\mathbf{m}))$ may be assumed to be small for $\mathbf{n}\neq\mathbf{m}$, we find further

$$\Big|\sum_{(j)}\Big|^2 \approx \sum_{\mathbf{n}}\Big|\sum_l\phi_l^*(\mathbf{X}-\mathbf{r}_0(\mathbf{n}))\phi_l(\mathbf{X}'-\mathbf{r}_0(\mathbf{n}))\Big|^2. \quad (59)$$

Substituting (59) into (51) we obtain

$$\begin{aligned} C^{\nu\mu\bar{\nu}\bar{\mu}}_{\mathbf{h}\mathbf{g}\bar{\mathbf{h}}\bar{\mathbf{g}}} &= L(\mathbf{k}_0^{\mu*}+\bar{\mathbf{k}}_0^{\bar{\mu}*}-\mathbf{k}_0^{\nu}-\bar{\mathbf{k}}_0^{\bar{\nu}})F(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) \\ &\times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\cdot\mathbf{r}(\mathbf{0})\} \\ &-2\sum_{\mathbf{n}}\iint_{\text{crystal}} d\mathbf{X}d\mathbf{X}'\Big|\sum_l\phi_l^*(\mathbf{X}-\mathbf{r}_0(\mathbf{n}))\phi_l(\mathbf{X}'-\mathbf{r}_0(\mathbf{n}))\Big|^2 \\ &\times \exp 2\pi i\{(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*})\cdot\mathbf{X}'-(\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\cdot\mathbf{X}\} \\ &\approx L(\mathbf{k}_0^{\mu*}+\bar{\mathbf{k}}_0^{\bar{\mu}*}-\mathbf{k}_0^{\nu}-\bar{\mathbf{k}}_0^{\bar{\nu}}) \\ &\times \{F(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})-H(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\} \\ &\times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\cdot\mathbf{r}(\mathbf{0})\}, \end{aligned} \quad (60)$$

where

$$\begin{aligned} H(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) &= h(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) \\ &\times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\cdot\mathbf{r}_0\} \end{aligned} \quad (61)$$

and

† $\delta_{\zeta\zeta'}$ equals 1 for $\zeta=\zeta'$ and equals 0 for $\zeta\neq\zeta'$.

$$h(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = 2\iint d\mathbf{X}\,d\mathbf{X}'\Big|\sum_l \phi_l^*(\mathbf{X})\phi_l(\mathbf{X}')\Big|^2 \times \exp 2\pi i\{(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}).\mathbf{X}'-(\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}).\mathbf{X}\}\,. \quad (62)\dagger$$

The integrations in (62) are over the whole space and the notation $\mathbf{r}_0$ in (61) is the position of the atom relative to the lattice point, $\mathbf{r}_0 = \mathbf{r}_0(\mathbf{0})-\mathbf{r}(\mathbf{0})$.‡

Writing

$$S(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = F(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})-H(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\,, \quad (63)$$

we finally find the result (52). The ordinary crystal structure factor F can be constructed from the atomic scattering factor as

$$F(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = f(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) \times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}).\mathbf{r}_0\}\,. \quad (64)$$

Substituting (61) and (64) into (63), we have

$$S(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = s(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) \times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}).\mathbf{r}_0\}\,, \quad (65)$$

where

$$s(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = f(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})-h(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}})\,. \quad (66)$$

The factor s may be called *the atomic scattering factor for Kikuchi patterns.*

In cases where the unit cell contains many atoms, (65) is generalized approximately as follows:

$$S(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = \sum_k s_k(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) \times \exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}).\mathbf{r}_k\}\,, \quad (67)$$

where s_k is the atomic scattering factor for Kikuchi patterns of the kth atom in the unit cell and $\mathbf{r}_k$ is the position of the kth atom relative to the lattice point, namely $\mathbf{r}_k = \mathbf{r}_k(\mathbf{0})-\mathbf{r}(\mathbf{0})$. Thus the crystal structure factor for Kikuchi patterns is constructed from the atomic scattering factors for Kikuchi patterns by a similar procedure as in the construction of the ordinary crystal structure factor.

(B) *Use of Thomas–Fermi model*

Here the atomic scattering factor for Kikuchi patterns is evaluated by the use of the Thomas–Fermi model of atoms. Heisenberg (1931) has given the following expression in his treatment of inelastic scattering of X-rays by atoms:

$$\sum_l \phi_l^*(\mathbf{X})\phi_l(\mathbf{X}') = \frac{1}{h^3}\int_{|\mathbf{p}|\leqq P_0} d\mathbf{p}\exp\left\{2\pi i\frac{\mathbf{p}}{h}.(\mathbf{X}-\mathbf{X}')\right\}, \quad (68)$$

where $\mathbf{p}$ is the momentum vector, and P_0, the maximum value of $|\mathbf{p}|$, is given by

$$P_0 = \sqrt{[2me\{\Phi(r_1)-\Phi_0\}]}\,, \quad (69)$$

where $-e\Phi$ is the potential energy of an electron in the spherical atom, $-e\Phi_0$ is its maximum energy, and

$$r_1 = |\mathbf{X}_1| \quad \text{and} \quad \mathbf{X}_1 = \tfrac{1}{2}(\mathbf{X}+\mathbf{X}')\,. \quad (70)$$

Writing

$$\mathbf{X}_2 = \mathbf{X}-\mathbf{X}' \quad (71)$$

and substituting (68) into (62), we have

$$\begin{aligned} h(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) &= 2\iint d\mathbf{X}_1\,d\mathbf{X}_2\exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}).\mathbf{X}_1\} \\ &\quad\times\exp\{-2\pi i.\tfrac{1}{2}(\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}+\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}).\mathbf{X}_2\} \\ &\quad\times\frac{1}{h^6}\iint_{|\mathbf{p}|,|\mathbf{p}'|\leqq P_0(\mathbf{X}_1)} d\mathbf{p}\,d\mathbf{p}'\exp\left\{2\pi i\frac{(\mathbf{p}-\mathbf{p}')}{h}.\mathbf{X}_2\right\} \\ &\approx 2\int d\mathbf{X}_1\exp\{2\pi i(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}).\mathbf{X}_1\} \\ &\quad\times\frac{4\pi}{3h^3}\left\{P_0(\mathbf{X}_1)-\frac{h}{4}|\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}+\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}|\right\}^2 \\ &\quad\times\{P_0(\mathbf{X}_1)+\frac{h}{8}|\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}+\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}|\}\,. \end{aligned} \quad (72)\dagger$$

Writing

$$h(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = Zh^\circ(u,v)\,, \quad (73)$$

where Z is the atomic number of the atom, we obtain

$$h^\circ(u,v) = \int_0^{R_0} R_1^2\,dR_1\left\{\left(\frac{\varphi}{R_1}\right)^{\frac{1}{2}}-v\right\}^2\left\{\left(\frac{\varphi}{R_1}\right)^{\frac{1}{2}}+\frac{v}{2}\right\}\frac{\sin uR_1}{uR_1}\,, \quad (74)\ddagger$$

where

$$\varphi(R_0)/R_0 = v^2\,, \quad (75)$$

$$u = 2\pi a|\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}| \quad (76)$$

and

$$v = \pi b|\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}+\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}|\,, \quad (77)$$

with the abbreviations

$$2\pi a = 2\pi\left(\frac{3}{32\pi^2}\right)^{\frac{1}{3}}\frac{h^2}{2me^2}\frac{1}{Z^{\frac{1}{3}}} = \frac{2{\cdot}94}{Z^{\frac{1}{3}}}\,\text{Å} \quad (78)$$

† X and X′ in (62) are used respectively in place of $\mathbf{X}-\mathbf{r}_0(\mathbf{n})$ and $\mathbf{X}'-\mathbf{r}_0(\mathbf{n})$ in (60).

‡ The same expressions (60), (61) and (62) can be obtained when $\Psi_0(\mathbf{q})$ in (43) is formed by setting up an antisymmetrical determinant of atomic functions instead of the Bloch functions.

† If $\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}$ and $\mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}$ are real, $\approx$ in (72) is replaced by $=$.

‡ The detailed derivation of (72) and (74) are not given here. Compare the derivation of (20), (23) in Heisenberg's article (Heisenberg, 1931) and that of the second equation in Bewilogua's paper (Bewilogua, 1931).

and

$$\pi b = \frac{\pi a}{(6\pi Z)^{\frac{1}{3}}} = \frac{0{\cdot}553}{Z^{\frac{1}{3}}}\text{ Å}\,. \tag{79}$$

$\varphi(R_1)$ in (74) is given by

$$\varphi(R_1) = \frac{r_1}{Ze}\{\Phi(r_1)-\Phi_0\}\,, \tag{80}$$

where

$$R_1 = r_1/a\,. \tag{81}$$

The atomic scattering factor is given by

$$f(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*}-\mathbf{k}_{\mathbf{h}}^{\nu}-\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = Zf^{\circ}(u) \tag{82}$$

(Debye, 1930), where

$$f^{\circ}(u) = \int_0^{\infty}\left(\frac{\varphi}{R_1}\right)^{\frac{3}{2}}\frac{\sin uR_1}{uR_1}R_1^2dR_1\,. \tag{83}$$

Thus the atomic scattering factor for Kikuchi patterns is given by

$$s(\mathbf{k}_{\mathbf{g}}^{\mu*}+\bar{\mathbf{k}}_{\bar{\mathbf{g}}}^{\bar{\mu}*},\ \mathbf{k}_{\mathbf{h}}^{\nu}+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}^{\bar{\nu}}) = Z\{f^{\circ}(u)-h^{\circ}(u,v)\}\,. \tag{84}$$

The function $\{f^{\circ}(u)-h^{\circ}(u,v)\}$ signifies the atomic scattering factor for Kikuchi patterns divided by the atomic number. The numerical value of this function is given in Table 1 and Fig. 2.

Table 1. *Values of* $\{f^{\circ}(u)-h^{\circ}(u,v)\}$

v \ u	0·0†	0·4	1·0	2·2
0·00	0·000	0·000	0·000	0·000
0·05	0·319			
0·10	0·486			
0·20	0·674	0·410	0·175	0·049
0·30	0·776			
0·40	0·839	0·572	0·299	0·098
0·50	0·880			
0·60	0·909	0·639	0·362	0·144
0·70	0·929			
0·80	0·944	0·673	0·395	0·171
0·90	0·954			
1·00	0·963	0·692	0·413	0·188
∞	1·000	0·725	0·446	0·220

† Values given by Bewilogua (1931).

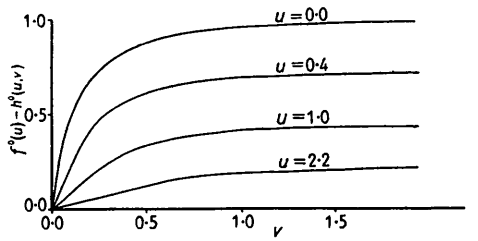

Fig. 2.

At $u = 0$ this function becomes

$$[f^{\circ}(u)-h^{\circ}(u,v)]_{u=0} = 1-\int_0^{R_0}\left\{\left(\frac{\varphi}{R_1}\right)^{\frac{1}{2}}-v\right\}^2\left\{\left(\frac{\varphi}{R_1}\right)^{\frac{1}{2}}+\frac{v}{2}\right\}R_1^2dR_1 = S_i(v)/Z\,, \tag{85}$$

and s reduces to S_i/Z, where $S_i(v)$ is the function given by Heisenberg (1931). As v tends to infinity, $h^{\circ}(u,v)$ tends to zero and

$$\lim_{v\to\infty}[f^{\circ}(u)-h^{\circ}(u,v)] = f^{\circ}(u)\,. \tag{86}$$

Then s tends to the ordinary atomic scattering factor f.

5. Examples; transmission through a parallel-sided crystal

In this section we apply the theory to the case of transmission through a thin crystal slab of area $|N_1\mathbf{a}_1\times N_2\mathbf{a}_2|$ and thickness $(N_3\mathbf{a}_3\cdot\mathbf{b}_3)/|\mathbf{b}_3|$.

(*A*) *General background*

Let us first consider the case where the incident wave and reciprocal wave do not suffer Bragg reflexions in the crystal. Then we may take Φ_0 and $\bar{\Phi}_0$ to be finite and all the other Φ's and $\bar{\Phi}$'s to be zero. Thus from (53) we obtain

$$J(r_A) \propto \frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_0,\ \mathbf{k}_0+\bar{\mathbf{k}}_0)}{(\mathbf{k}_0+\bar{\mathbf{k}}_0)^4}\bar{\Phi}_0\bar{\Phi}_0^*L(\mathbf{0})\,. \tag{87}$$

In this expression

$$\bar{\Phi}_0 = \sqrt{\{\bar{\Gamma}_0/\bar{\gamma}_0\}}\bar{\Phi}_0^{(v)}\,, \tag{88}$$

where $\bar{\Phi}_0^{(v)}$ is the amplitude of the reciprocal wave in free space, $\bar{\gamma}_0$ is the normal component of the wave vector $\bar{\mathbf{k}}_0$, $\bar{\Gamma}_0$ is the normal component of the wave vector in free space and

$$L(\mathbf{0}) = N_1N_2N_3\,. \tag{89}$$

Substituting (88) and (89) into (87), we obtain

$$J(\mathbf{r}_A) \propto \frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_0,\ \mathbf{k}_0+\bar{\mathbf{k}}_0)}{(\mathbf{k}_0+\bar{\mathbf{k}}_0)^4}\frac{\bar{\Gamma}_0}{\bar{\gamma}_0}N_1N_2N_3\,. \tag{90}$$

By the use of (67), (84) and (85), we have

$$S(\mathbf{k}_0+\bar{\mathbf{k}}_0,\ \mathbf{k}_0+\bar{\mathbf{k}}_0) = \sum_k s_k(\mathbf{k}_0+\bar{\mathbf{k}}_0,\ \mathbf{k}_0+\bar{\mathbf{k}}_0) = \sum_k S_{ik}(v_k)\,,$$

where the suffix k denotes the quantities related to the kth atom in the unit cell. Except for the effect of refraction, $\bar{\Gamma}_0/\bar{\gamma}_0$, the result (90) agrees with the common expectation that the intensity of inelastic scattering by an assembly of atoms is simply the sum of intensities of inelastic scattering by the component atoms. It is clear that (90) corresponds to Kikuchi's divergent secondary wave mentioned in our introduction and gives the monotonicly decreasing background of the diffraction pattern.

(*B*) *Kikuchi lines and bands*

Let us next consider the case where the reciprocal wave is reflected by a net plane $\bar{\mathbf{H}}$, while the incident

wave does not suffer any Bragg reflexion. Adopting the first approximation by Bethe (1928), we may take Φ_0, $\bar{\Phi}'_0$, $\bar{\Phi}''_0$, $\bar{\Phi}'_{\bar{\mathbf{H}}}$ and $\bar{\Phi}''_{\bar{\mathbf{H}}}$ to be finite and all the other Φ's and $\bar{\Phi}$'s to be zero, since higher approximations make calculations only more complicated and the essential nature of the Kikuchi patterns is determined by the first approximation.

Assuming that

$$S(\mathbf{k}_0+\bar{\mathbf{k}}^{\bar{\mu}}_{\bar{\mathbf{g}}},\ \mathbf{k}_0+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}}) \approx S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{g}}},\ \mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{h}}}) \quad (91)$$

and

$$(\mathbf{k}_0+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})^2 \approx (\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{h}}})^2, \quad (92)$$

where $\bar{\mathbf{k}}_{\bar{\mathbf{h}}}$ is the arithmetic mean of $\bar{\mathbf{k}}'_{\bar{\mathbf{h}}}$ and $\bar{\mathbf{k}}''_{\bar{\mathbf{h}}}$, we obtain, as in (A),

$$J(\mathbf{r}_A) \propto \sum_{\bar{\mathbf{h}},\bar{\mathbf{g}}} \frac{S(\mathbf{k}_0+\bar{\mathbf{k}}^{\bar{\mu}}_{\bar{\mathbf{g}}},\ \mathbf{k}_0+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})}{(\mathbf{k}_0+\bar{\mathbf{k}}^{\bar{\nu}}_{\bar{\mathbf{h}}})^2(\mathbf{k}_0+\bar{\mathbf{k}}^{\bar{\mu}}_{\bar{\mathbf{g}}})^2} \sum_{\bar{\nu},\bar{\mu}} \bar{\Phi}^{\bar{\nu}}_{\bar{\mathbf{h}}} \bar{\Phi}^{\bar{\mu}*}_{\bar{\mathbf{g}}} \times L(\bar{\mathbf{k}}^{\bar{\mu}}_0-\bar{\mathbf{k}}^{\bar{\nu}}_0) \exp\{2\pi i(\bar{\mathbf{k}}^{\bar{\mu}}_0-\bar{\mathbf{k}}^{\bar{\nu}}_0).\mathbf{r}(0)\}, \quad (93)$$

where

$$\begin{aligned} &L(\bar{\mathbf{k}}^{\bar{\mu}}_0-\bar{\mathbf{k}}^{\bar{\nu}}_0) \exp\{2\pi i(\bar{\mathbf{k}}^{\bar{\mu}}_0-\bar{\mathbf{k}}^{\bar{\nu}}_0).\mathbf{r}(0)\} \\ &= \sum_{\mathbf{n}} \exp\{2\pi i(\bar{\mathbf{k}}^{\bar{\mu}}_0-\bar{\mathbf{k}}^{\bar{\nu}}_0).(\mathbf{n}+\mathbf{r}(0))\} \\ &= N_1N_2 \sum_{n_3=0}^{N_3-1} \exp\{2\pi i(\bar{\gamma}^{\bar{\mu}}_0-\bar{\gamma}^{\bar{\nu}}_0)\frac{\mathbf{b}_3}{|\mathbf{b}_3|}.(n_3\mathbf{a}_3+\mathbf{r}(0))\}. \end{aligned} \quad (94)$$

If the origin of the coordinates is assumed to lie on the lower surface of the crystal, i.e. the surface nearer the photographic plate, and the arbitrary vector $\mathbf{r}(0)$ is taken to satisfy the relation

$$\mathbf{r}(0).\mathbf{b}_3 = \tfrac{1}{2}, \quad (95)$$

then, with the sufficient approximation

$$\sin Nx/\sin x \approx \sin Nx/x,$$

the summation term in (94) is reduced to

$$\sum_{n_3=0}^{N_3-1} \approx \exp\{\pi i(\bar{\gamma}^{\bar{\mu}}_0-\bar{\gamma}^{\bar{\nu}}_0)D\} \frac{\sin\{\pi(\bar{\gamma}^{\bar{\mu}}_0-\bar{\gamma}^{\bar{\nu}}_0)D\}}{\pi(\bar{\gamma}^{\bar{\mu}}_0-\bar{\gamma}^{\bar{\nu}}_0)D/N_3}, \quad (96)$$

where

$$D = N_3\mathbf{a}_3 \cdot \mathbf{b}_3/|\mathbf{b}_3|. \quad (97)$$

According to the dynamical theory presented by Bethe (1928), we have

$$\bar{\gamma}'_0-\bar{\gamma}''_0 = \frac{|U_{-\bar{\mathbf{H}}}|}{\sqrt{\{\bar{\gamma}_0\bar{\gamma}_{\bar{\mathbf{H}}}\}}} \sqrt{\{1+\bar{W}^2\}}, \quad (98)$$

where

$$U_{-\bar{\mathbf{H}}} = (2me/h^2)V_{-\bar{\mathbf{H}}}. \quad (99)$$

Here the $V_{\bar{\mathbf{h}}}$'s are given by the Fourier expansion of $V_{00}(\mathbf{r})$

$$V_{00}(\mathbf{r}) = -e\sum_{\bar{\mathbf{h}}} V_{\bar{\mathbf{h}}} \exp(-2\pi i\bar{\mathbf{h}}.\mathbf{r}). \quad (100)$$

The quantity $\bar{W}$ is a parameter appearing in Bethe's dynamical theory in order to represent the deviation from the Bragg condition. According to the same theory, the amplitudes are given as

$$\left.\begin{aligned} \bar{\Phi}'_0 &= \tfrac{1}{2}\left(1-\frac{\bar{W}}{\sqrt{\{1+\bar{W}^2\}}}\right)\sqrt{\left\{\frac{\bar{\Gamma}_0}{\bar{\gamma}_0}\right\}}\,\bar{\Phi}^{(r)}_0, \\ \bar{\Phi}''_0 &= \tfrac{1}{2}\left(1+\frac{\bar{W}}{\sqrt{\{1+\bar{W}^2\}}}\right)\sqrt{\left\{\frac{\bar{\Gamma}_0}{\bar{\gamma}_0}\right\}}\,\bar{\Phi}^{(r)}_0, \\ \bar{\Phi}'_{\bar{\mathbf{H}}} &= \tfrac{1}{2}\frac{U^*_{-\bar{\mathbf{H}}}}{|U_{-\bar{\mathbf{H}}}|}\frac{1}{\sqrt{\{1+\bar{W}^2\}}}\sqrt{\left\{\frac{\bar{\Gamma}_0}{\bar{\gamma}_{\bar{\mathbf{H}}}}\right\}}\,\bar{\Phi}^{(v)}_0, \\ \bar{\Phi}''_{\bar{\mathbf{H}}} &= -\tfrac{1}{2}\frac{U^*_{-\bar{\mathbf{H}}}}{|U_{-\bar{\mathbf{H}}}|}\frac{1}{\sqrt{\{1+\bar{W}^2\}}}\sqrt{\left\{\frac{\bar{\Gamma}_0}{\bar{\gamma}_{\bar{\mathbf{H}}}}\right\}}\,\bar{\Phi}^{(v)}_0. \end{aligned}\right\} \quad (101)$$

Since Z is proportional to f in most cases, we have a rough estimate

$$\frac{F(\bar{\mathbf{H}})}{|F(\bar{\mathbf{H}})|}.\frac{U_{-\bar{\mathbf{H}}}}{|U_{-\bar{\mathbf{H}}}|} \approx 1. \quad (102)$$

Since s is proportional to f for large v, we have

$$S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}},\ \mathbf{k}_0+\bar{\mathbf{k}}_0) \sim F(\bar{\mathbf{H}}),$$

and this relation holds approximately in most experimental cases. Thus we find

$$\frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}},\ \mathbf{k}_0+\bar{\mathbf{k}}_0)}{|S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}},\ \mathbf{k}_0+\bar{\mathbf{k}}_0)|}\frac{U_{-\bar{\mathbf{H}}}}{|U_{-\bar{\mathbf{H}}}|} \sim 1. \quad (103)$$

Finally, by the help of (94), (96), (98), (101) and (103), (93) turns out to be

$$\begin{aligned} J(\mathbf{r}_A) \propto{}& \frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_0,\ \mathbf{k}_0+\bar{\mathbf{k}}_0)}{(\mathbf{k}_0+\bar{\mathbf{k}}_0)^4}\frac{\bar{\Gamma}_0}{\bar{\gamma}_0}N_1N_2N_3 \\ &+\left[\left\{\frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}},\ \mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}})}{(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}})^4}\frac{\bar{\Gamma}_0}{\bar{\gamma}_{\bar{\mathbf{H}}}} - \frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_0,\ \mathbf{k}_0+\bar{\mathbf{k}}_0)}{(\mathbf{k}_0+\bar{\mathbf{k}}_0)^4}\frac{\bar{\Gamma}_0}{\bar{\gamma}_0}\right\}\right. \\ &\left.\times\frac{1}{2(1+\bar{W}^2)} - \frac{|S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}},\ \mathbf{k}_0+\bar{\mathbf{k}}_0)|}{(\mathbf{k}_0+\bar{\mathbf{k}}_0)^2(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}})^2}\frac{\bar{\Gamma}_0}{\sqrt{[\bar{\gamma}_0\bar{\gamma}_{\bar{\mathbf{H}}}]}}\frac{\bar{W}}{(1+\bar{W}^2)}\right] \\ &\times N_1N_2N_3\left[1-\frac{\sin\{2\pi D|U_{-\bar{\mathbf{H}}}|\sqrt{[1+\bar{W}^2]}/\sqrt{[\bar{\gamma}_0\bar{\gamma}_{\bar{\mathbf{H}}}]}\}}{2\pi D|U_{-\bar{\mathbf{H}}}|\sqrt{[1+\bar{W}^2]}/\sqrt{[\bar{\gamma}_0\bar{\gamma}_{\bar{\mathbf{H}}}]}}\right]. \end{aligned} \quad (104)$$

As the crystal becomes thicker, the oscillating term in the last bracket of (104) becomes smaller compared with 1, and (104) is reduced to

$$J(\mathbf{r}_A) \propto \left[\frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_0,\ \mathbf{k}_0+\bar{\mathbf{k}}_0)}{(\mathbf{k}_0+\bar{\mathbf{k}}_0)^4}\frac{\bar{\Gamma}_0}{\bar{\gamma}_0}+\left\{\frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}},\ \mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}})}{(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}})^4}\frac{\bar{\Gamma}_0}{\bar{\gamma}_{\bar{\mathbf{H}}}}-\frac{S(\mathbf{k}_0+\bar{\mathbf{k}}_0,\ \mathbf{k}_0+\bar{\mathbf{k}}_0)}{(\mathbf{k}_0+\bar{\mathbf{k}}_0)^4}\frac{\bar{\Gamma}_0}{\bar{\gamma}_0}\right\}\frac{1}{2(1+\overline{W}^2)}-\frac{|S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}},\ \mathbf{k}_0+\bar{\mathbf{k}}_0)|}{(\mathbf{k}_0+\bar{\mathbf{k}}_0)^2(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}})^2}\frac{\bar{\Gamma}_0}{\sqrt{[\bar{\gamma}_0\bar{\gamma}_{\bar{\mathbf{H}}}]}}\frac{\overline{W}}{(1+\overline{W}^2)}\right] N_1N_2N_3. \tag{105}$$

The first term of (105), as shown in § 5(A), gives the general background (Kikuchi's divergent secondary wave) at point A, i.e. in the direction $-\bar{\mathbf{k}}_0$.

When the geometrical position of a Kikuchi line predicted by the elementary theory lies near the incident spot, we have $|\mathbf{k}_0+\bar{\mathbf{k}}_0| \ll |\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}}|$ if we take point A on the line as is shown in Fig. 3. If we take

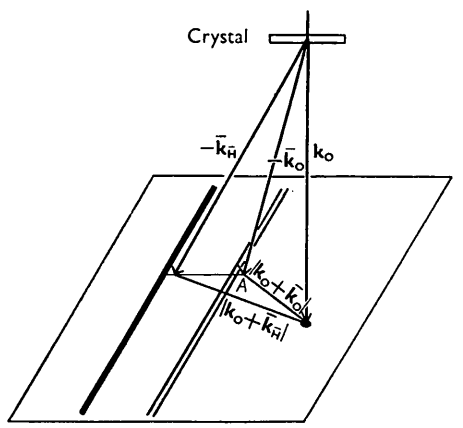

Fig. 3.

point A on the other line of the pair shown in Fig. 3, we have $|\mathbf{k}_0+\bar{\mathbf{k}}_0| \gg |\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}}|$. In both cases the second term in (105) prevails over the third. The second term of (105) can be interpreted in accordance with the intuitive explanation given by Kikuchi (1928) as follows: When point A lies on the geometrical position of a Kikuchi line, then a part of the divergent secondary wave in the direction $-\bar{\mathbf{k}}_0$ is reflected by the net plane $-\overline{\mathbf{H}}$, as is shown in Fig. 4, and the intensity at point A, $J(\mathbf{r}_A)$, is decreased. At the same time it is increased because a part of the divergent secondary wave in the direction $-\bar{\mathbf{k}}_{\bar{\mathbf{H}}}$ is reflected by the same net plane into the direction $-\bar{\mathbf{k}}_0$. The factor $1/\{2(1+\overline{W}^2)\}$ on the right-hand side of the curly bracket in (105) means the averaged reflexion power of net plane $-\overline{\mathbf{H}}$ for a plane wave. The first term in the curly bracket is the intensity of the divergent secondary wave (divided by $N_1N_2N_3$) in the direction $-\bar{\mathbf{k}}_{\bar{\mathbf{H}}}$; the second in $-\bar{\mathbf{k}}_0$. Therefore, the entire second term of (105), the curly bracket multiplied by $1/\{2(1+\overline{W}^2)\}$, gives the net intensity which follows as the result of the decrease and the increase of $J(\mathbf{r}_A)$ mentioned above. The second term of (105) becomes negative for $|\mathbf{k}_0+\bar{\mathbf{k}}_0| < |\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}}|$ and positive for $|\mathbf{k}_0+\bar{\mathbf{k}}_0| > |\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}}|$. This means that the line nearer the incident spot is white (defect) and the other is black (excess). Thus the second term of (105) corresponds to the Kikuchi line. It is symmetric in $\overline{W}$, as shown in Fig. 5(a), and the breadth of the lines is given by $-1 \leqq \overline{W} \leqq +1$. This breadth is proportional to $|U_{-\bar{\mathbf{H}}}|$.

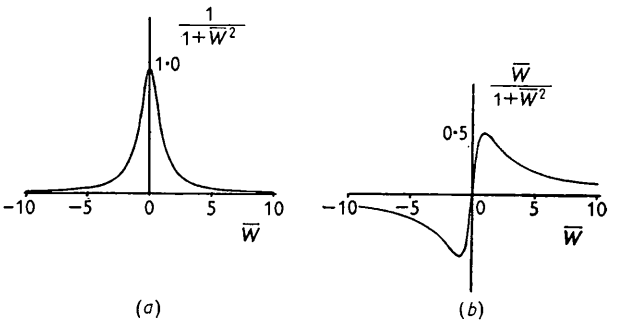

Fig. 5.

When the incident spot falls near the middle of the pair of lines, and point A lies near the geometrical position of a Kikuchi line, we have $|\mathbf{k}_0+\bar{\mathbf{k}}_0| \approx |\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}}|$. The third term in (105) prevails over the second. The third term is antisymmetric in $\overline{W}$, as is shown in Fig. 5(b). Therefore, the third term of (105) gives a Kikuchi band. It is clear that this term becomes positive for $\overline{W} < 0$ inside the band and negative for $\overline{W} > 0$ outside the band. Thus the band is a black (excess) one. The occurrence of a Kikuchi band cannot be interpreted in an elementary way because the third term involves $S(\mathbf{k}_0+\bar{\mathbf{k}}_{\bar{\mathbf{H}}}, \mathbf{k}_0+\bar{\mathbf{k}}_0)$, which is irreducible to the simple sum of S_{ik}'s and is derived only by the help of the reciprocity theorem.

In intermediate cases in which the second and the third terms in (105) are comparable, a superposition of a pair of lines and a band appears.

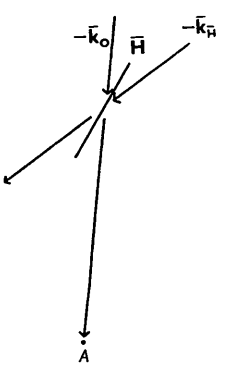

Fig. 4.

The above mentioned properties of (105) are in agreement with experimental observations except for a group of observations discussed in § 6(*B*). Thus the deficiency of Laue's original theory (1935) is completely eliminated.

The oscillating term in the last bracket of (104), which becomes observable in the case of thin crystals, accounts for the fine structure of Kikuchi patterns as actually observed for thin crystals of molybdenite (Uyeda, Fukano & Ichinokawa, 1954). This fine structure may be interpreted in an elementary way as follows: Let us assume a crystal to have a simple lattice and to contain only one kind of atom. The atoms lie in the depths D_n from the surface nearer the photographic plate, where $D_n = (n+\frac{1}{2})D/N_3$ and where $n = 0, 1, \ldots, N_3-1$. A divergent secondary wave is assumed to be emitted by an atom lying at depth D_n. Let us adopt here the elementary assumption, according to Kikuchi, that the secondary divergent wave is a superposition of plane waves. Then both parts of the divergent wave which propagate in the directions $-\bar{\mathbf{k}}_{\mathbf{0}}$ and $-\bar{\mathbf{k}}_{\bar{\mathbf{H}}}$ are reflected by the net plane $-\bar{\mathbf{H}}$ throughout the crystal layer which lies nearer the photographic plate and has a thickness D_n, if point A lies on the geometrical position of a Kikuchi line. But for a plane wave of wave vector $-\bar{\mathbf{k}}_{\mathbf{0}}$ or $-\bar{\mathbf{k}}_{\bar{\mathbf{H}}}$ falling on a crystal plate of thickness D_n, the reflexion power is

$$\sin^2 \{\pi U_{\bar{\mathbf{H}}}/[1+\overline{W}^2]D_n/|[\bar{\gamma}_{\mathbf{0}}\bar{\gamma}_{\bar{\mathbf{H}}}]\}/(1+\overline{W}^2) \quad (106)$$

according to the ordinary dynamical theory of diffraction (Uyeda, Ichinokawa & Fukano, 1954). If this reflexion power is averaged over all possible thicknesses D_n, the average of (106) is

$$\begin{aligned}
&\frac{1}{N_3}\sum_{n=0}^{N_3-1} \sin^2 \{\pi U_{\bar{\mathbf{H}}}/[1+\overline{W}^2]D_n/|[\bar{\gamma}_{\mathbf{0}}\bar{\gamma}_{\bar{\mathbf{H}}}]\}/(1+\overline{W}^2) \\
&= \frac{1}{2(1+\overline{W}^2)}\frac{1}{N_3}\left[N_3 - \sum_{n=0}^{N_3-1}\cos\{2\pi U_{\bar{\mathbf{H}}}/[1+\overline{W}^2] \times (n+\tfrac{1}{2})D/N_3|[\bar{\gamma}_{\mathbf{0}}\bar{\gamma}_{\bar{\mathbf{H}}}]\}\right] \\
&\approx \frac{1}{2(1+\overline{W}^2)}\left[1 - \frac{\sin 2\pi U_{\bar{\mathbf{H}}}/[1+\overline{W}^2]D/|[\bar{\gamma}_{\mathbf{0}}\bar{\gamma}_{\bar{\mathbf{H}}}]}{2\pi U_{\bar{\mathbf{H}}}/[1+\overline{W}^2]D/|[\bar{\gamma}_{\mathbf{0}}\bar{\gamma}_{\bar{\mathbf{H}}}]}\right]. \quad (107)
\end{aligned}$$

This expression coincides with the oscillating term of (104), which is produced by the secondary divergent waves emitted by all the atoms in the crystal.* This interpretation may be said to give the physical meaning of the fine structure of the Kikuchi pattern, and it makes clear the reason for the difference of the fine structures of Kikuchi patterns and of Kossel–Möllenstedt patterns.

The intensity distribution along the lines and band has not been discussed; but, if required, it can be calculated from (104) and (105).

* Although the oscillating term (107) gives not only the fine structure of Kikuchi lines but also that of Kikuchi bands, the interpretation given here is valid only for Kikuchi lines.

6. Discussion

(*A*) *Effect of imperfections*

In the present work the author assumes that the cause of the divergent wave which results in Kikuchi patterns is inelastic scattering. It is possible, however, that the scattering at lattice imperfections, such as lattice vibrations, dislocations and impurities, can also cause divergent waves, even though the scattering is elastic. In some crystals, the effect of imperfections may not be overlooked. Since strong Kikuchi patterns are produced by crystals, such as diamonds, which have only a few imperfections, it may be said that inelastic scattering is the main cause of Kikuchi patterns. An experimental proof of this fact was recently given by Boersch (1953). He showed, by applying his electron filter, that the Kikuchi pattern from mica is due to inelastic scattering.

The intensity of the Kikuchi pattern may increase with the presence of imperfections so long as the geometrical position of the pattern is undisturbed. The theoretical calculation of the effect is not here worked out, but it can be done in principle by using the generalized reciprocity theorem [§ 2(*B*)], provided the nature of the imperfection is known.

It must be stated that the effect of lattice vibrations should be taken into account when calculating the structure amplitudes for Kikuchi patterns and the Fourier coefficients of the elastic potential field.

(*B*) *Effect of absorption*

While the present theory should eliminate the difficulties which appear in the case of reflexion patterns and in cases where the incident wave suffers Bragg reflexions or where the reciprocal wave suffers simultaneous reflexions (Kikuchi envelopes), there are some experimental observations which we suppose cannot be explained by our theory. Among them are those of Shinohara & Matsukawa (1933), Boersch (1937) and Pfister (1953), who observed that Kikuchi bands in transmission patterns change from defect to excess, or vice versa, with the change of the energy of the incident electrons and with the change of the thickness of the crystal. Alam, Blackman & Pashley (1954) observed a similar effect for the intensities of Kikuchi bands in reflexion patterns when the angle of incidence is changed. The failure of the present theory to cover these observations is due to our assumption that $\varphi_i(\mathbf{r})$ is very small compared with $\varphi_0(\mathbf{r})$. In the above observations the Kikuchi pattern predominates over the Laue spots. In such cases our assumption that $\varphi_i(\mathbf{r})$ is very small compared with $\varphi_0(\mathbf{r})$ does not apply. To explain these observations, the effect of absorption must be taken into account (Pfister, 1953; Kainuma, 1953) and we have not concerned ourselves with absorption.

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A Magneto-X-ray Study of Magnetite at 78°K.*

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The X-ray diffraction pattern produced by a small single crystal of magnetite after cooling through the transition at 119° K. has been examined. It is demonstrated, by using orientated magnetic fields during the cooling process, that up to six different domain orientations are present in the crystal at 78° K. This number of domain orientations can be produced only if the symmetry of the low-temperature phase of magnetite is orthorhombic or lower.

Introduction

The crystal structure of magnetite, Fe_3O_4, below its transition at 119° K. has recently attracted considerable interest. Verwey & Haayman (1941) suggested that magnetite has the inverse spinel structure at room temperature and that the transition is due to an ordering of the ferrous and ferric ions in the octahedral positions of the spinel lattice. This ordered arrangement, Verwey, Haayman & Romeijn (1947) proposed, possesses orthorhombic symmetry.§ Measurements of the deformation of circular disks cooled through the transition in a magnetic field, by strain-gauge techniques (Bickford, 1953), were consistent with an orthorhombic structure, and it has been shown that

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§ The cell they gave was tetragonal, but it really has orthorhombic symmetry.