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On the Inelastic Scattering of Electron in Crystal

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The inelastic and coherent scattering of electron arising from the non-conservation of momentum is discussed. For electron diffraction, the subsidiary maxima are theoretically obtained in the Kikuchi pattern. The intensity distribution in the microscopic image of bright field shows the fringes and is antisymmetric with respect to the exact Bragg position. In the dark field case, the intensity distribution is symmetric.

The inelastic scattering, which was discussed by Kainuma[1] and Takagi[2] on the Kikuchi patterns, is of general importance in electron diffraction. The appearance of the subsidiary maxima in the Kikuchi patterns which was observed by Uyeda et al[3] revealed that the inelastically scattered wave shows the coherent phenomena. Recently, Kamiya and Uyeda[4] also showed that the inelastic waves make the microscopic image as like as that due to the elastic wave. We may consider that the coherent interference of inelastically scattered wave arises mainly from the non-conservation of momentum of electron. In the present paper, we shall reexamin the inelastic scattering of an electron by a crystal and study its effect on the electron diffraction and microscopic image.

The wave function of the total system is given by

$$\Psi = c_{kN}\Psi_k\Phi_N e^{-(i/\hbar)(E_k+E_N)t} + \sum_{k'N'}\Big(\sum_{g'} c_{k'N'}^{g'}\Psi_{k'}^{g'}\Big)\Phi_{N'}e^{-(i/\hbar)(E_{k'}+E_{N'})t}, \quad (1)$$

where the first and second terms are the wave functions of initial and final states, and Ψ_k and Φ_N are those of the electron and the crystal, respectively. The wave function of the electron in crystal in its initial state is written as

$$\Psi_k = \frac{1}{\sqrt{V}}\sum_i \alpha_i \sum_h \phi_h{}^i \exp(i\boldsymbol{k}_h{}^i\cdot\boldsymbol{r}), \quad (2)$$

in which V is the volume of the crystal, $\sum_h \phi_h{}^i\phi_h{}^{j*}=\delta_{ij}$, and α_i should be determined by the usual boundary condition at the entrance surface. The wave fields are numbered by i. On the other hand, as the wave function of the secondary electron we take the following orthogonal system

$$\Psi_{k'}^{g'} = \frac{1}{\sqrt{V}}\sum_{i'}\alpha_{i'}^{g'}\sum_{h'}\phi_{h'}^{i'}\exp(i\boldsymbol{k}'^{i'}_{h'}\cdot\boldsymbol{r}), \quad (3)$$

in which $\alpha_{i'}^{g'}$ is determined by the following boundary condition at the exit surface,

$$\left.\begin{aligned} &\sum_{i'}\alpha_{i'}^{g'}\sum_{h'}\phi_{h'}^{i'}\exp(ik'^{i'}_{h'\nu}D)=\delta_{h'g'}\exp(iK'_{g'\nu}D) \\ &\text{and} \\ &\qquad \boldsymbol{k}'^{i'}_{g'\tau}=\boldsymbol{k}'_{g'\tau}, \end{aligned}\right\} \quad (4)$$

where D is the thickness of the parallel sided crystal, $\boldsymbol{K}$ the wave vector of electron in vacuum, and τ and ν indicate the tangential and normal components, respectively.

If the matrix element of the interaction between the crystal states $\Phi_{N'}$ and Φ_N is written as

$$(N'|H'|N)=\sum_l A_{NN',l}(\boldsymbol{q})\exp i(\boldsymbol{b}_l+\boldsymbol{q})\boldsymbol{r}, \quad (5)$$

the first order coefficient of $c_{k'N'}^{g'}$ is given by

$$\begin{aligned} c_{k'N'(1)}^{g'} &= -\frac{1}{\hbar}(k'N'|H'|kN)_{g'}\frac{e^{(i/\hbar)\Delta Et}-1}{\Delta E} \\ &= \frac{1}{\hbar}\sum_{h,h'}A_{NN',g+h'-h}(\boldsymbol{q})\sum_{i,i'}\alpha_i\phi_h{}^i\alpha_{i'}^{g'*}\phi_{h'}^{i'*} \\ &\quad\times\frac{e^{i\Delta k_q^{ii'}D}-1}{\Delta k_q^{ii'}}\frac{e^{(i/\hbar)\Delta Et}-1}{\Delta E}\delta'_{k_{0\tau},k_{0\tau}+b_{g\tau}-q_\tau}, \end{aligned} \quad (6)$$

where

$$\Delta k_q^{ii'} = k_{0\nu}^i + b_{g\nu} + q_\nu - k'^{i'}_{0\nu},$$
$$\Delta E = E_N + E_k - E_{N'} - E_{k'}$$

and

$$\boldsymbol{b}_g = \boldsymbol{b}_h + \boldsymbol{b}_l - \boldsymbol{b}_{h'}.$$

If the momentum is conserved, i.e. $\Delta k_q^{ii'}=0$, the waves belonging to the different wave fields are incoherent except accidental cases, since the wave vectors $k_{h'}^{\prime i'}$ are limited by the energy conservation. As the other origin of the inelastic coherent scattering, we may consider the non-conservation of energy which is concerned with the life times of excited states of the crystal and the duration of interaction between the electron and crystal. In general, however, it may not be necessary to take these factors into account. In this case, the intensity of the g'-reflection is given by

$$J_{g'}=\left(\frac{mV}{2\pi h^2}\right)^2\frac{k'}{K}\times\int|(k'N'|H'|kN)_{g'}|^2\rho(q_\nu)dq_\nu\,. \quad (7)$$

In the following, we shall consider the case $g'=0$, and we put

$$B_{ii'}=\sum_{h,h'}A_{NN',g+h'-h}(\boldsymbol{q})\alpha_i\psi_h{}^i\alpha_i^{0*}\psi_{h'}^{i'*}\,. \quad (8)$$

In the case where the primary and secondary waves excite the h- and h'-reflections, respectively, and the two-wave approximation applied to each wave, we have

$$\begin{aligned}B_{11'}=\frac{1}{4}\Big\{&A_g\left(1-\frac{W}{\sqrt{1+W^2}}\right)\left(1-\frac{W'}{\sqrt{1+W'^2}}\right)\\&+A_{g+h'}\left(1-\frac{W}{\sqrt{1+W^2}}\right)\frac{e^{-i\varphi_{h'}}}{\sqrt{1+W'^2}}\\&+A_{g-h}\frac{e^{i\varphi_h}}{\sqrt{1+W^2}}\left(1-\frac{W'}{\sqrt{1+W'^2}}\right)\\&+A_{g+h'-h}\frac{e^{i\varphi_h}}{\sqrt{1+W^2}}\frac{e^{-i\varphi_{h'}}}{\sqrt{1+W'^2}}\Big\}\\&\times\exp\left[i(k_{0\nu}^{\prime i'}-K'_{0\nu})D\right]\end{aligned} \quad (9)$$

etc. Here, W and W' are "Selektionsfehler" for the primary and secondary waves, respectively, $A_l\equiv A_{NN'l}(\boldsymbol{q})$, and φ_h the argument of the Fourier potential v_h. If we assume that A_l and the Fourier potentials are all real and $\rho(q_\nu)=D/2\pi$, we obtain

$$\begin{aligned}\int|(k'N'|H|kN)|^2\rho(q_\nu)dq_\nu=&\sum_{i,i'}b_{ii'}^2\\&+2(b_{11'}b_{21'}+b_{12'}b_{22'})\frac{\sin(dD/2)}{dD/2}\\&+2(b_{11'}b_{12'}+b_{21'}b_{22'})\frac{\sin(d'D/2)}{d'D/2}\\&+2b_{11'}b_{22'}\frac{\sin\{(d-d')D/2\}}{(d-d')D/2}\\&+2b_{12'}b_{21'}\frac{\sin\{(d+d')D/2\}}{(d+d')D/2}\,,\end{aligned} \quad (10)$$

in which $b_{ii'}$ is the absolute value of $B_{ii'}$ and d and d' are given by

$$\left.\begin{aligned}d&=k_0{}^1-k_0{}^2=\frac{v_h}{k}\sqrt{1+W^2}\,,\\d'&=k_0^{\prime 1'}-k_0^{\prime 2'}=\frac{v_{h'}}{k'}\sqrt{1+W'^2}\,.\end{aligned}\right\} \quad (11)$$

We now consider the case of $W\to\infty$, i.e. the primary wave does not excite any Bragg reflection. Then, (10) becomes

$$A_g{}^2+\left\{\frac{1}{2}(A_{g+h'}^2-A_g{}^2)\frac{1}{1+W'^2}-A_gA_{g+h'}\times\frac{W'}{1+W'^2}\right\}\left(1-\frac{\sin(d'D/2)}{d'D/2}\right). \quad (12)$$

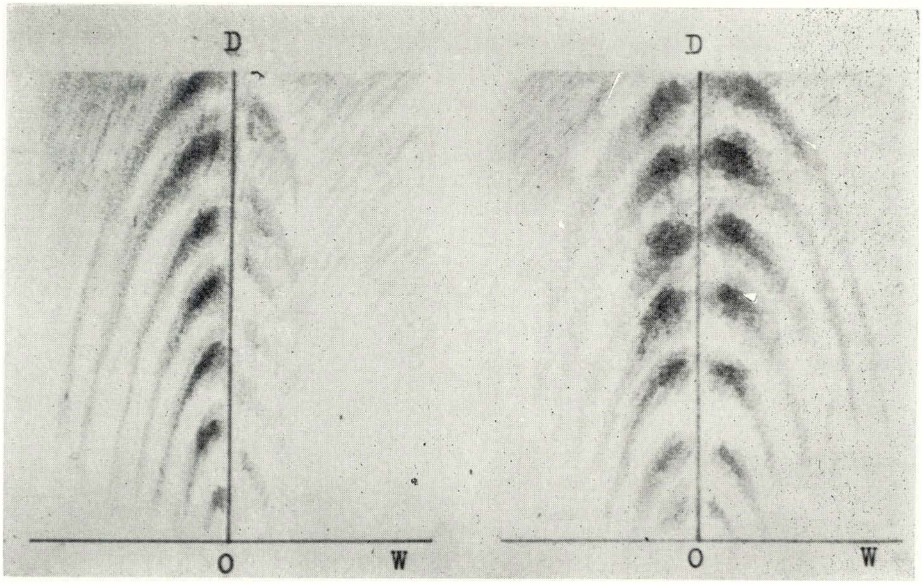
The intensity obtained from (12) is similar to that of the Kikuchi pattern, and the oscillating factor gives the subsidiary maxima. When the thickness is large, this factor becomes independent of W' and the subsidiary maxima vanish.

In the case of the microscopic image, we should integrate (10) over the objective aperture. Such an integration is, however, difficult, since $A_g(\equiv A_{NN',g}(\boldsymbol{q}))$ is a function of W' and depends on the process of inelastic scattering. For simplicity, we consider the case where the objective aperture is so small that (10) is regarded as constant within the aperture.

The case of the microscopic image of bright field may be regarded as that of $W=W'$, $g'=0$ and $h=h'$. Then, (10) is reduced to

$$\begin{aligned}a_0{}^2+2a_h&\left\{a_h\left(\frac{W}{1+W^2}\right)^2-a_0\frac{W}{1+W^2}\right\}\\&\times\left(1-\frac{\sin(dD/2)}{dD/2}\right)-\frac{1}{2}a_h{}^2\left(\frac{W}{1+W^2}\right)^2\\&\times\left(1-\frac{\sin(dD)}{dD}\right).\end{aligned} \quad (13)$$

where $a_g=A_gS$, S being the solid angle of the objective aperture. In this formula, the intensity obtained from the second term is antisymmetric with respect to W as well as the Kikuchi pattern, and the period of the equi-thickness fringe is equal to that due to the elastic waves. The third term is symmetric with respect to W and the period is half of the former, but the intensity may be much weaker than that due to the second term, since the maximum value of the coefficient of the oscillating factor is one twelfth of the second term for $a_0=a_h$.



(a) (b)

Fig. 1. Intensity distribution in microscope image made by inelastic wave.
a) Bright field, b) Dark field.
$(A_0, A_h > 0)$

In a similar manner to the case of (13) the formula of the microscopic image of dark field is given by

$$a_h^2\left\{1-2\left(\frac{W}{1+W^2}\right)^2\left(1-\frac{\sin(dD/2)}{dD/2}\right)\right.$$
$$\left.+\frac{1}{2}\left(\frac{W}{1+W^2}\right)^2\left(1-\frac{\sin(dD)}{dD}\right)\right\}. \tag{14}$$

In this formula, the intensity is symmetric with respect to W and is different from that of the bright field. The intensity distributions in the images of bright and dark fields are shown in Fig. 1 (a) and (b), respectively.

The experimental verification of these results was shown by Kamiya and Uyeda[5].

The details will be published in J. Phys. Soc. Japan.

References

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4 Y. Kamiya and R. Uyeda: J. Phys. Soc. Japan **16** (1961) 1361.
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DISCUSSION

S. MIYAKE: I understand that the inelastic scattering can give many kinds of interference patterns. Still, I should like to ask, if your theory could explain the experimental result of Kamiya and Uyeda on the equal thickness fringes in images of magnesium oxide crystal, in which the fringes due to inelastic scattering appear *exactly* at the same positions as those due to elastic scattering.

Y. KAINUMA: Yes, by our theory it can be shown that the fringes due to inelastic scattering appear at the same positions as those due to elastic scattering, and it was the first aim of this study to explain such a behaviour. However, the fact that the observed intensity decreases with thickness at larger thickness could not be explained yet at the present stage of our theory. Such a phenomenon would be explained by taking account of the secondary process of inelastic scattering.