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Anoamlous Intensity of Mirror Reflection from the Surface of a Single Crystal

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Systematic observations are made on the well known intensity enhancement of mirror reflection which is observed when the mirror spot comes on a Kikuchi line. It is found that the anomalous enhancement appears only when the mirror spot lies on a part of the Kikuchi line forming a Kikuchi envelope and the existence of a diffracted wave nearly parallel to the surface plays an essential part in the phenomenon. In such a case, the two-wave approximation is not valid. A wave equation of four waves is'solved and the intensity of the mirror reflection is calculated by using an electronic computer. The result explains satisfactorily the obseved intensity anomaly.

1. Recently quite many important studies have been made intensively on electron diffraction phenomena, but most of them are concerned with the Laue case, and very few with the Bragg case. Among the phenomena of the Bragg case, some phenomena, which have been well known for a long time, have remained not completely explained. The present problem is one of this kind.

As will be seen later, this phenomenon has some features which are not seen in ordinary diffraction phenomena. Firstly, the intensity of mirror reflection which is usually neglected is just the subject of consideration. Secondly, because the direction of the diffracted wave is nearly parallel to the surface, the wave field is expected to be peculiar and different from both the ordinary Bragg case and the Laue case. Thirdly, this phenomenon can be explained only by taking account of several waves even at the stage of the first approximation, although only one diffracted wave is expected from geometrical consideration.

Many years ago Kikuchi and Nakagawa[1] observed that mirror reflection becomes quite strong when it coincides with an oblique Kikuchi line. Later Miyake, Kohra and Takagi studied this pheomenon experimentally, and took notice that the direction of the diffracted wave is nearly parallel to the surface. They considered the mechanism of the anomalous intensity of mirror reflection in the following way: the diffracted wave nearly parallel to the surface suffers from zig-zag reflection among atomic planes parallel to the surface, which have a high potential barrier and a small spacing. Owing to this situation and to the refractive index of the crystal the diffracted wave or reflected-back wave can not go out of the crystal. As a result, the incident energy is reflected back from the surface as the mirror reflection.

In this report a more exact analysis of the experimental condition for appearance

Fig. 1. A photograph from a cleavage of a rock salt crystal.

of the anomalous mirror reflection will be given and the wave equation will be numerically solved using an electronic computor to calculate the intensity and to study the wave field.

2. The condition of anomalous mirror reflection was studied systematically for the diffraction patterns from cleavage faces of several crystals of zincblende and rock salt. An example of the photographs from a rock salt crystal is given in Fig. 1, where the mirror reflection is found on an oblique Kikuchi line. It is noticed here that not only the mirror reflection is strong but also other diffraction patterns, such as Kikuchi lines and especially diffuse spots, are quite intense as has previously been observed by Miyake[2].

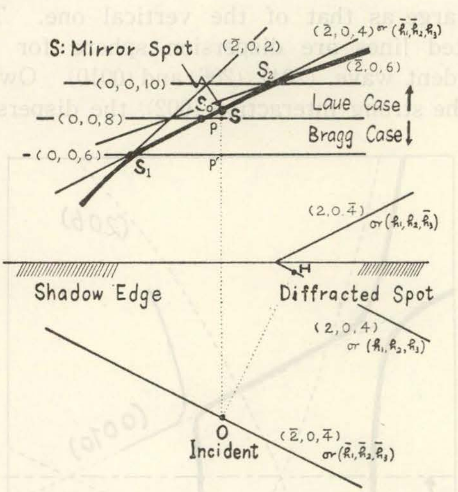

Fig. 2. Schematic diagram of a diffraction pattern.

In Fig. 2 a schematic diagram of the diffraction pattern from a rook salt crystal is given. Here, for convenience, the effects of absorption and refraction are neglected, and some patterns which cannot be observed are drawn. We suppose that the mirror spot lies on a Kikuchi line ($\bar{2}04$), or ($\bar{h}_1\bar{h}_2h_3$), where the $x-y$ plane is taken to be the surface and the z-axis directs inwards. Because the cleavage face is generally a mirror plane of the crystals, the incident spot must lie on the Kikuchi line ($\bar{2}0\bar{4}$) or ($\bar{h}_1\bar{h}_2\bar{h}_3$), which is the mirror image of the Kikuchi line in question with respect to the shadow edge. This means that when the mirror spot lies on the Kikuchi line ($\bar{2}04$), the diffraction takes place on the plane (204) and diffraction spot must be found on the line (204). According to Miyake, Kohra and Takagi[3], the diffraction spot is expected to lie very close to the shadow edge, when the intensity enhancement appears. In other words, the diffraction beam is nearly parallel to the surface.

Let us consider the phenomenon in more detail. The Kikuchi line ($\bar{2}04$) in question is intersected at two points S_1 and S_2 with other Kikuchi lines, say, ($\bar{2}02$) and ($\bar{2}06$). These form the so-called Kikuchi envelope. Besides, there are horizontal Kikuchi lines, say, (004), (006) and (008), intersecting the oblique Kikuchi line ($\bar{2}04$) at S_1, S_0 and S_2, respectively.

According to our systematic observations, the intensity enhancement takes place only if the mirror spot lies approximately inside the region S_1S_2, that is, on a part of the Kikuchi envelope. From a geometrical consideration, it is seen that the z-component of the wave vector of the diffracted wave, $\boldsymbol{k}_{hz}$, can be determined directly from the distance between the mirror spot and the horizontal Kikuchi line (006) by the relation

$$k_{hz}=\overrightarrow{\mathrm{SP}}\cdot b_{001}/\overline{\mathrm{PP}'}, \tag{1}$$

where b_{001} is the reciprocal vector for (001). If S is above S_0, we have $k_{hz}>0$ (Laue case) and if S below S_0, $k_{hz}<0$ (Bragg case). For the region between S_1 and S_2 we have

$$|k_{hz}|\leq b_{001}. \tag{2}$$

This is the necessary and sufficient condition for the anomalous mirror reflection. Usually we have

$$b_{001}\lesssim\sqrt{v_0}\,. \tag{3}$$

where v_0 is the mean inner potential multiplied by $8\pi^2 m/h^2$.

The relation (2) makes the two-wave approximation to be not valid as will be seen later. The relation (3) means that the diffracted wave cannot go out of the crystal because of the refraction effect, and is also essential for the appearance of the anomalous mirror reflection.

3. Now we consider which waves are strong under the above condition. In Fig. 3 the Ewald diagram is shown where (204) or ($h_1h_2h_3$) reflection takes place. The cross section is normal to the surface and involves the lattice point ($h_1h_2h_3$). The amplitudes of

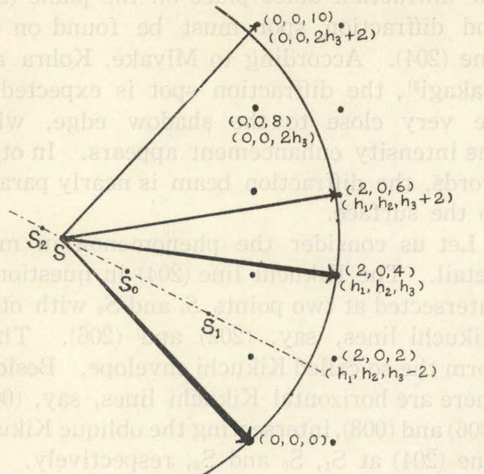

Fig. 3. Ewald diagram.

other waves are given as the second approximation by

$$\frac{v_g\phi_0+v_{g-h}\phi_h}{\kappa^2-k_g^2}\ . \qquad (4)$$

As seen from the diagram, points $(h_1h_2h_3\pm 2)$ are very close to the Ewald sphere, and accordingly for these points $\kappa^2-k_g^2$ are very small, and v_{g-h} are now v_{002} or $v_{00\bar{2}}$ which are the largest Fourier coefficients. Accordingly these amplitudes must be large. This means that the diffracted waves $(h_1h_2h_3\pm 2)$ are further reflected on the net plane (002) parallel to the surface into $(h_1h_2h_3\pm 2)$. Through these waves, other waves $(002h_3)$ and $(002_3\pm 2)$ will become large. Thus we must consider all or some of them, at least two waves, as the first approximation, besides the incident and (204) waves. For example, in the case of $|k_{hz}|\sim b_{001}(h=204)$, we may well choose four waves, ϕ_0, ϕ_{204}, ϕ_{206} and ϕ_{0010}, as strong ones. The corresponding wave equation is

$$\begin{pmatrix} \kappa^2-k_0^2 & v_{\bar{2}0\bar{4}} & v_{\bar{2}0\bar{6}} & v_{00\bar{1}\bar{0}} \\ v_{204} & \kappa^2-k_{204}^2 & v_{00\bar{2}} & v_{\bar{2}0\bar{6}} \\ v_{206} & v_{002} & \kappa^2-k_{062}^2 & v_{20\bar{4}} \\ v_{0010} & v_{\bar{2}06} & v_{\bar{2}04} & \kappa^2-k_{0010}^2 \end{pmatrix}\begin{pmatrix} \phi_0 \\ \phi_{204} \\ \phi_{206} \\ \phi_{0010} \end{pmatrix}=0. \qquad (5)$$

As pointed out by Lamla,[4] the secular equation of (5) has four independent eigen values, two out of which are adopted here as justified in a later paragraph.

The boundary conditions are given for both tangential components of wave vectors respectively as follows:

$$\left.\begin{aligned} 1+\Psi_0&=\sum_{i=1,2} c^{(i)}(\phi_0{}^{(i)}+\phi_{0010}^{(i)}) \\ -\Gamma_0+\Gamma_0\Psi_0&=\sum_{i=1,2} c^{(i)}(\gamma_0{}^{(i)}\phi_0{}^{(i)}+\gamma_{0010}^{(i)}\phi_{0010}^{(i)}) \end{aligned}\right\} \qquad (6a)$$

and

$$\left.\begin{aligned} \Psi_h&=\sum_{i=1,2} c^{(i)}(\phi_{204}^{(i)}+\phi_{206}^{(i)}) \\ \Gamma_h\Psi_h&=\sum_{i=1,2} c^{(i)}(\gamma_{204}^{(i)}\phi_{206}^{(i)}+\gamma_{206}^{(i)}\phi_{206}^{(i)}) \end{aligned}\right\} \qquad (6b)$$

4. Numerical calculation were made using the electronic computor PC1, for the case where (204) reflection takes place for a zincblende crystal. As values of k_{hz} for which the Bragg-Laue condition is satisfied, two values $0.8b_{001}$ and $0.9b_{001}$ are assumed. In Fig. 4 the dispersion surface for $k_{hz}=0.8b_{001}$ is given, the cross section of which is the plane involving the incident plane. The scale of the horizontal axis is thirty times as large as that of the vertical one. The dotted lines are dispersion sphere for the incident wave, (204), (206) and (0010). Owing to the strong interaction (002), the dispersion

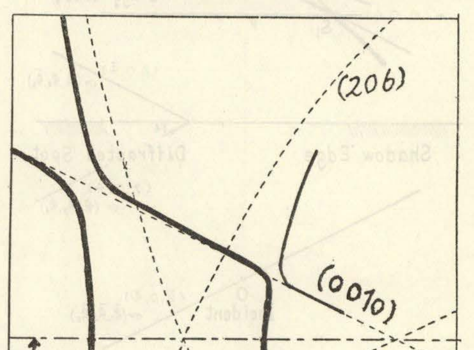

Fig. 4. Cross section of the dispersion surface

surface is pushed far away from the cross-point of the spheres (204) and (206). We are concerned with the regions of two branches I and II near the Laue point L_0 for which the Laue-Bragg condition on (204) is satisfied, and further only with the lower parts of the both branches below the horizontal line z', because

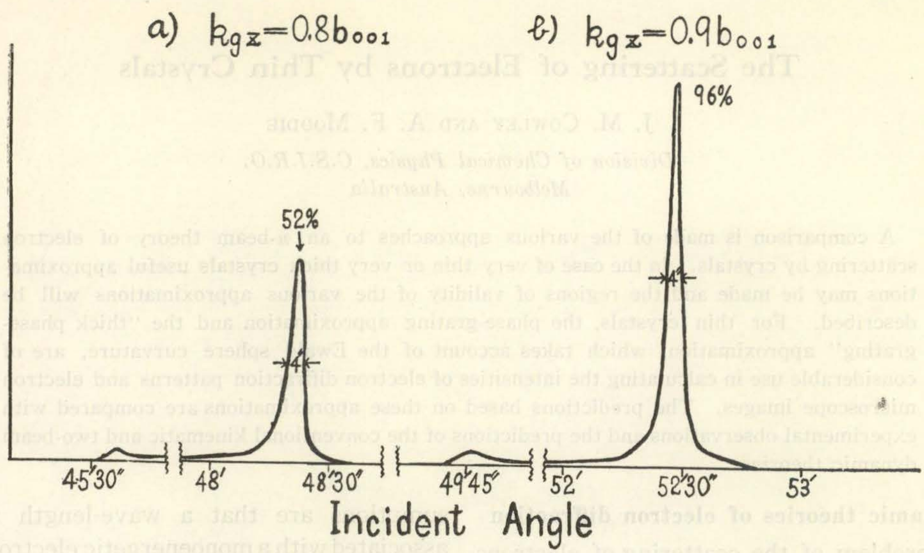

Fig. 5. Intensity curve of mirror reflection.

the energy flow vector belonging to these branches directs inwards or downwards. The ones belonging to the upper branches directs upwards while only the energy flow going inwards is allowed actually.

The intensity curve of the mirror reflection is shown in Fig. 5. The abscissa is the incident angle and its scale is exaggerated. The curve (a) is for $k_{hz}=0.8b_{001}$ and (b) for $k_{hz}=0.9b_{001}$. The reflection percent is about 50 and 95%, respectively. We can say that this explains the observed intensity enhancement satisfactorily. The intensity maximum appears in the neighbourhood of the Laue point L. According to the calculation, the wave field I is predominant and its wave point is imaginary. Among the partial waves of this wave field, (204) and (206) waves are predominant, and their wave vectors and amplitudes are conjugate to each other, respectively. Accordingly, these waves form a standing wave with respect to z-axis, which has a same period as that of (002) plane. Penetration depth of these waves is in the order of several Ångstrom. This shallow wave field will probably take an essential part in the intensity anomaly of mirror reflection as well as the characteristic brightness of whole diffraction pattern which take place with the enhancement of the mirror reflection[2].

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