Kikuchi pattern is accompanied by a few subsidiary maxima. This pattern is a superposition of a Kikuchi band and line, where the former predominates over the latter. Since the Kikuchi band has an asymmetric intensity near the position of the Bragg condition, the factor multiplying (1) is positive for positive N's and negative for negative N's. Therefore, the conditions (2a) and (2b) must be used respectively for positive and negative N's. Assuming these conditions, we analysed the pattern. The thickness of the film Md calculated from any successive subsidiary maxima was almost constant and the mean value turned out to be $Md = 520$ Å. This is in agreement with the thickness calculated from the $(21\bar{3}0)$-K.–M. pattern by the ordinary procedure. The values of $|V_{20\bar{2}2}|$ calculated from each maximum, even if showing rather large fluctuations, gave the mean value $|V_{20\bar{2}2}| = 1$ volt. This is in agreement with the theoretical value $|V_{20\bar{2}2}| = 1{\cdot}2$ volts. It should be noted here that if equation (3) of the previous paper is used instead of (1), $|V_{20\bar{2}2}|$ turns out to be imaginary if we assign to N the values 1, 2, 3 as given in the figure, and to be more than 10 volts if we assign the values **2**, **3**, **4**. Similar agreement was also obtained in the case of some other indices. These facts may prove that we are here without doubt dealing with the subsidiary maxima of the interference function of Kikuchi patterns.

The reason that the subsidiary maxima are not observable in parallel-beam diffraction patterns may be as follows: The irradiated area of specimens in this case is much larger (usually $\gtrsim 100\,\mu$ diameter) than in the case of a divergent beam (usually $\lesssim 5\,\mu$ diameter). If crystals are thin enough to produce subsidiary maxima of resolvable angular widths, the curving of the crystal will, with larger irradiated area, inevitably disturb the appearance of Kikuchi pattern. It is worth mentioning that, contrary to the view held by early workers (Kikuchi, 1928), Kikuchi patterns appear even from quite thin crystals, if the irradiated area is reduced.

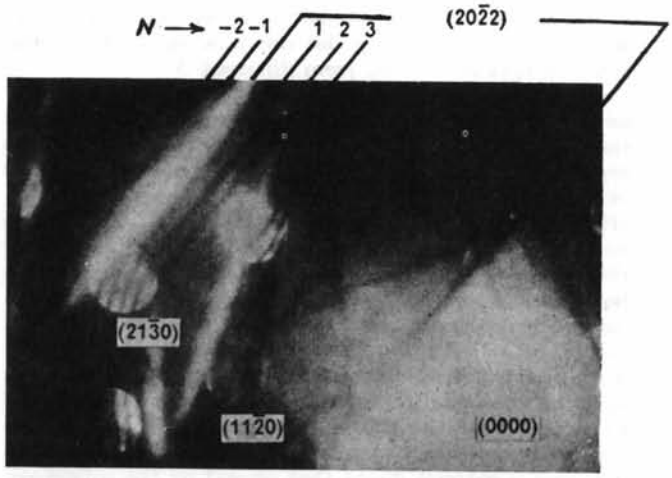

Fig. 1. Divergent-beam electron-diffraction pattern from a thin molybdenite film (520 Å).

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A dynamical theory of the simultaneous reflexion by two lattice planes. I. Simple representation of the dispersion surface.

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The dispersion surface in reciprocal space plays an important role in the dynamical theory of X-ray and electron diffraction. To represent this surface graphically, a cross-section with a plane is often used (e.g. Fues, 1939; Hoerni, 1950). In the present note, it will be shown that the theoretical formulation for the problem of simultaneous reflexion by two lattice planes, say with indices $h(h_1h_2h_3)$ and $h'(h_1'h_2'h_3')$, can be simplified by choosing a particular plane for the cross-section.

The Schrödinger equation for the electron with an energy eE in the periodic potential $V(\mathbf{r}) = \sum_h V_h \exp 2\pi i \mathbf{b}_h\mathbf{r}$, where $\mathbf{b}_h$ is the vector representing the reciprocal-lattice point, is

$$\Delta\psi + \frac{8\pi^2 me}{h^2}(E + V(\mathbf{r}))\psi = 0\,. \qquad (1)$$

Now ψ is considered to be composed of three waves corresponding to the indices 0, h and h', as follows:

$$\psi = u_0 \exp 2\pi i \mathbf{k}_0\mathbf{r} + u_h \exp 2\pi i \mathbf{k}_h\mathbf{r} + u_{h'} \exp 2\pi i \mathbf{k}_{h'}\mathbf{r}\,, \qquad (2)$$

where $\mathbf{k}_h = \mathbf{k}_0 + \mathbf{b}_h$, $\mathbf{k}_{h'} = \mathbf{k}_0 + \mathbf{b}_{h'}$; and u_0, u_h and $u_{h'}$ are the amplitudes of the plane waves. The three functions $\psi_m = \exp 2\pi i \mathbf{k}_m\mathbf{r}$ $(m = 0, h, h')$ are orthogonal to one another, as well as to the ψ_m's of indices other than 0, h and h'. Here we replace these three functions by

$$\varphi_0 = \psi_0, \quad \varphi_+ = \frac{1}{N}(\psi_h + c\psi_{h'}), \quad \varphi_- = \frac{1}{N}(c\psi_h - \psi_{h'}), \qquad (3)$$

where c is a constant, real and positive, and $N = \sqrt{(1+c^2)}$ is the normalizing factor. These functions are also orthogonal to one another, as well as to the ψ_m's of indices other than 0, h, and h'. ψ is rewritten as

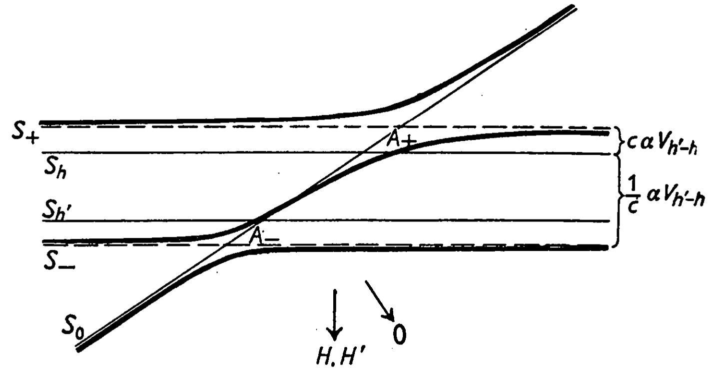

Fig. 1. Cross-section of dispersion surface by a c-plane for $c < 1$. HH' is perpendicular to the plane of the figure, H lying nearer to this plane than H'.

$$\psi = u_0\psi_0 + u_+\psi_+ + u_-\psi_- , \tag{4}$$

where

$$u_+ = N(u_h + cu_{h'}) , \quad u_- = N(cu_h - u_{h'}) . \tag{5}$$

For brevity we put

$$\varkappa^2 = \frac{2me}{h^2}(E+V_0) ,$$

$$x_0 = \varkappa - |\mathbf{k}_0| , \; x_h = \varkappa - |\mathbf{k}_h| , \; x_{h'} = \varkappa - |\mathbf{k}_{h'}| ,$$

and

$$\alpha = \frac{1}{2\varkappa}\frac{2me}{h^2} .$$

Let us assume, among x_h, $x_{h'}$ and c, a relation

$$x_{h'} - x_h = \alpha V_{h'-h}(c-1/c) , \tag{6}$$

wherein $V_{h'-h}$ is taken to be real and positive by a proper choice of the coordinate origin. Then the homogenous equations for u_0, u_+ and u_-, which can be obtained by applying the usual procedure utilizing (1) and the orthogonal relations among the ψ_m's, is reduced to an especially simple form:

$$\begin{pmatrix} x_0 & \frac{\alpha}{N}(V_h^* + cV_{h'}^*) & \frac{\alpha}{N}(cV_h^* - V_{h'}^*) \\ \frac{\alpha}{N}(V_h + cV_{h'}) & x_h + c\alpha V_{h'-h} & 0 \\ \frac{\alpha}{N}(cV_h - V_{h'}) & 0 & x_h - \frac{1}{c}\alpha V_{h'-h} \end{pmatrix} \begin{pmatrix} u_0 \\ u_+ \\ u_- \end{pmatrix} = 0 . \tag{7}$$

The compatibility relation of (7) is given by

$$x_0 = \frac{\left|\frac{\alpha}{N}(V_h + cV_{h'})\right|^2}{x_h + c\alpha V_{h'-h}} + \frac{\left|\frac{\alpha}{N}(cV_h - V_{h'})\right|^2}{x_h - \frac{1}{c}\alpha V_{h'-h}} . \tag{8}$$

The ratios of the amplitudes of the waves are obtained from (7) as

$$\frac{u_+}{u_0} = -\frac{\frac{\alpha}{N}(V_h + cV_{h'})}{x_h + c\alpha V_{h'-h}} , \quad \frac{u_-}{u_0} = -\frac{\frac{\alpha}{N}(cV_h - V_{h'})}{x_h - \frac{1}{c}\alpha V_{h'-h}} , \tag{9}$$

so that, from (5),

$$\frac{u_h}{u_0} = -\frac{1}{N}\left(\frac{\frac{\alpha}{N}(V_h + cV_{h'})}{x_h + c\alpha V_{h'-h}} + c\frac{\frac{\alpha}{N}(cV_h - V_{h'})}{x_h - \frac{1}{c}\alpha V_{h'-h}}\right) ,$$

$$\frac{u_{h'}}{u_0} = -\frac{1}{N}\left(c\frac{\frac{\alpha}{N}(V_h + cV_{h'})}{x_h + c\alpha V_{h'-h}} - \frac{\frac{\alpha}{N}(cV_h - V_{h'})}{x_h - \frac{1}{c}\alpha V_{h'-h}}\right) . \tag{10}$$

As readily known from the geometrical meaning of x_h and $x_{h'}$, the surface in the reciprocal space represented by (6), for a given value of c, is approximately a plane perpendicular to the line joining the reciprocal points $H(h_1h_2h_3)$ and $H'(h_1'h_2'h_3')$. We call it the c-plane. Equation (8) gives a curve which corresponds to the cross-section of the dispersion surface by this plane. Fig. 1 shows the form of this curve. The lines S_0, S_h and $S_{h'}$ are the cross-sections of the spheres with radius $\varkappa$ having the centres at O, H and H' respectively. S_h and $S_{h'}$ are parallel. The lines S_+ and S_- are parallel to S_h, lying outside and inside of the circle represented by S_h at the distances $c\alpha V_{h'-h}$ and $(1/c)\alpha V_{h'-h}$ respectively.

The cross-section of the dispersion surface is composed of three branches. It is apparent that they are, grossly speaking, made up by combining the two hyperbolae, around the centres A_+ and A_-, corresponding respectively to the first and second term in the right-hand side of (8); the lines S_0, S_+ and S_- are their asymptotes.

The above procedure can be applied in the same way to the cross-sections with the planes perpendicular to the lines joining the origin 0 and the points H or H'. It is not applicable in the case when the points 0, H and H' lie on a straight line.

For X-ray diffraction the construction can be carried out in an analogous way. This may be useful for the interpretation of the phenomena of simultaneous reflexion in X-ray and electron diffraction: for instance, those observed in Kossel patterns, Seemann patterns, Kikuchi lines, Kossel–Möllenstedt patterns, 'equal-inclination fringes' in electron-micrographs, and in the *Aufhellung* in rotation photographs, etc.

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