

upper layers, the intensities are measured with the normal-beam geometry and therefore the above considerations apply to them as well.

In addition to the discussed λ -independent solutions, equation (5) may have solutions dependent on the wavelength. This type of multiple diffraction may be called 'accidental' and its appearance in a particular case depends on the value of the wavelength used in the experiment. All techniques are affected by this kind of multiple diffraction, whose presence in a particular case can be ascertained by solving equation (5) or by a method like the one discussed by Speakman (1965).

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Dynamical Diffuse Scattering from Magnesium Oxide Single Crystals

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Effects of Bragg scattering on the distribution of diffuse scattering from single crystals of magnesium oxide have been studied in transmission electron-diffraction patterns. The crystals were in the form of thin plates with very uniform thickness. The patterns are explained from a theory which includes both Bragg scattering of the diffusely scattered waves (as in ordinary Kikuchi-line theory) and Bragg scattering of the incident wave; only single diffuse scattering has been considered, however.

Fine structure in the Kikuchi-line pattern is shown to depend on the excitation error of the corresponding reflexions, the amplitude of the fine-structure oscillations increasing as the Bragg condition is approached. Also the contribution of the non-oscillating part to the Kikuchi-line contrast was found to change with the reflexion condition of the incident beam. In this case the contrast decreases with decreasing excitation error of the reflexion. When many Bragg reflexions are strongly excited, as when the beam is close to a zone axis, the Kikuchi lines may vanish altogether, leaving a complicated fine structure pattern. Reversal of contrast along a Kikuchi line, from excess to defect, may also result from Bragg scattering of the incident beam. Effects of three- and four-beam interactions were frequently observed, and are discussed for a pattern of weak lines crossing a strong line pair. In addition to bending of the lines near intersections, line fragments which cannot be indexed as Kikuchi lines were found; these occur at a distance equal to a reciprocal lattice vector from an ordinary Kikuchi line, and are related to the Kikuchi envelope. In observation of Kikuchi bands it was found that, when the line pair was symmetrically disposed about the central spot, the individual Kikuchi lines were asymmetric, with the deficient part of the band profile inside the line pair. The contrast of these lines is discussed and is related to the interference form factor, $\langle f(s)f^*(s+h) \rangle$.

Introduction

The purpose of this paper is to present and discuss some dynamical effects in patterns of diffuse scattering from magnesium oxide single crystals; that is, effects

due to dynamical interactions with the Bragg scattering. Some of the patterns can be described as the transmission Kikuchi-line patterns which are explained in terms of a simple geometrical consideration given by Kikuchi; in others the excitation of Bragg reflexions by the incident beam leads to fine structure effects and contrast changes in Kikuchi lines which must be explained from the more complete theory of interactions between Bragg scattering and diffuse scattering.

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Such a treatment, in which Bragg scattering of both incident beam and the diffuse beams is taken into account, has been developed in recent years by Fukuhara (1963), Fujimoto & Kainuma (1963) and Gjønnes (1966). Below we shall adopt the notation and representation of the last reference.

General description of the patterns

Magnesium oxide crystals were prepared by burning magnesium metal in air in the usual way. The smoke was collected on a supporting carbon film. Along with the commonly occurring cube-shaped crystal, some thin rectangular $\{100\}$ plates about 1000 Å thick were also obtained. The plate-shaped crystals appeared from their electron micrographs (Fig. 1) to be perfectly plane parallel without defects. Selected area diffraction patterns from such crystals were taken in a JEM 6A electron microscope using a tilting stage. Usually the grids were oriented in the holder so that the carbon film was below the specimen.

The transmission diffraction patterns (Figs. 2–6) showed complicated fine structures in the diffuse scattering; Kikuchi lines with good contrast appeared for lines of quite high indices. Owing to the uniform thickness, conditions were favourable for recording fine structure effects in the Kikuchi-line pattern.

The fine structure was found to depend on the diffraction condition of the incident beam; as a rule, no fine structure was observed for Kikuchi lines when the corresponding Bragg reflexions were not excited by the incident beam. When the corresponding reflexion was excited, a quite extensive fine structure accompanied the Kikuchi band or line, as already shown in Fig. 5 of a previous paper (Gjønnes, 1966). Other examples are shown in Figs. 2 and 3, where again the 002 and $00\bar{2}$ reflexions are excited. The intensity oscillations in the fine structure were largest when the incident beam satisfied the Bragg condition for the corresponding reflexion, as can be seen in these patterns. For intermediate values of the excitation error, the fine structure appeared mainly in the region between the Kikuchi line and the adjacent Bragg or direct spot.

Also the non-oscillating contribution to the Kikuchi line seemed to depend on the excitation error of the reflexion, in agreement with the theory (Gjønnes, 1966); *i.e.* the line contrast vanished as the Bragg condition of the corresponding reflexion was approached (Figs. 3 and 4). When several Bragg reflexions were strongly excited, as when the incident beam was near a zone axis, a pattern of complicated fine structure which was quite unlike a normal Kikuchi-line pattern, was obtained (Fig. 5).

Effects of three, or more, beam interactions were frequently apparent, especially near Kikuchi-line intersections. In Figs. 2 and 3 appreciable bending of the weak 82/ deficient lines is seen where they cross the broad 002 and $00\bar{2}$ lines. Several line fragments which cannot be indexed as Kikuchi lines are also observed

in this region. They appear at $\mathbf{s}+\mathbf{h}$, where \mathbf{s} corresponds to a Kikuchi-line position and \mathbf{h} is the 002 reciprocal lattice vector. We may thus call them *displaced Kikuchi lines*. Schematic representation of the pattern in Fig. 2 is shown in Fig. 9(b), where the displaced Kikuchi lines, 82/′, are indicated by broken lines, and dotted lines show the Kikuchi-line positions expected from the simple geometrical consideration of the Kikuchi line. Here it should be noted that the diffraction condition in Figs. 2 and 3 is the same as the condition which produces the Kikuchi envelope; *i.e.* the excess 82/ lines which are not seen on the plates should form the envelope. The 820 line is seen to be doubled in the region inside the 002 line pair. Similar doubling or broadening was in general found when a weak deficient line crossed a strong line pair at right angles.

A rather similar, but more complicated pattern which includes the 42/ lines is shown in Fig. 4. Here several of the corresponding Bragg reflexions are excited, and fine structure appears in connection with some of the lines. We may note that the ± 002 lines cannot be seen at all, apart from the fine structure around lines through the Bragg and direct spots. It is seen that the contrast of the 422 lines is reversed from defect to excess on crossing the ± 420 lines.

Asymmetric Kikuchi lines bounding a Kikuchi band were observed when the line pair was nearly symmetrically disposed about the incident beam, but the deficient part of the asymmetric profile was found to be closest to the central spot (Fig. 6), contrary to the normal Kikuchi-band contrast.

Discussion

In this section we shall discuss the observations outlined above on the basis of the general theory of interaction between diffuse and Bragg scattering developed by Fujimoto & Kainuma (1963), and Gjønnes (1966). Following the approach and notation of the latter reference, we shall represent the amplitude of diffuse scattering towards $\mathbf{k}_0+\mathbf{s}+\mathbf{h}$, where \mathbf{k}_0 is the wave vector of the incident beam, \mathbf{s} a scattering vector (usually taken within the first Brillouin zone of the projection) and \mathbf{h} a reciprocal lattice vector, as a sum over triple scattering processes described by products of three operators:

$$S(2)_{hg}f(\mathbf{s}+\mathbf{g}-\mathbf{g}')S(1)_{g'0}. \quad (1)$$

These three operators represent, from right to left, Bragg scattering of the incident beam, from \mathbf{k}_0 to $\mathbf{k}_0+\mathbf{g}'$, diffuse scattering from $\mathbf{k}_0+\mathbf{g}'$ to $\mathbf{k}_0+\mathbf{g}+\mathbf{s}$, Bragg scattering of the diffuse wave along $\mathbf{k}_0+\mathbf{g}+\mathbf{s}$ to $\mathbf{k}_0+\mathbf{h}+\mathbf{s}$.

The diffuse scattering will be considered to decrease rapidly with \mathbf{s} , as is the case for inelastic scattering; consequently we may restrict attention to terms where $\mathbf{g}=\mathbf{g}'$, except when *e.g.* $|\mathbf{s}|$ and $|\mathbf{s}-\mathbf{h}|$ are nearly equal as when the Kikuchi lines are symmetrically disposed about the central beam.

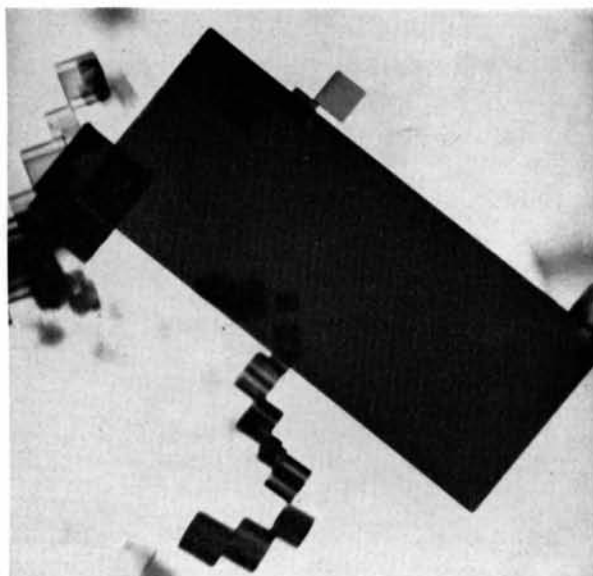


Fig.1. Electron microscope image of magnesium oxide plate ($\times 90000$).

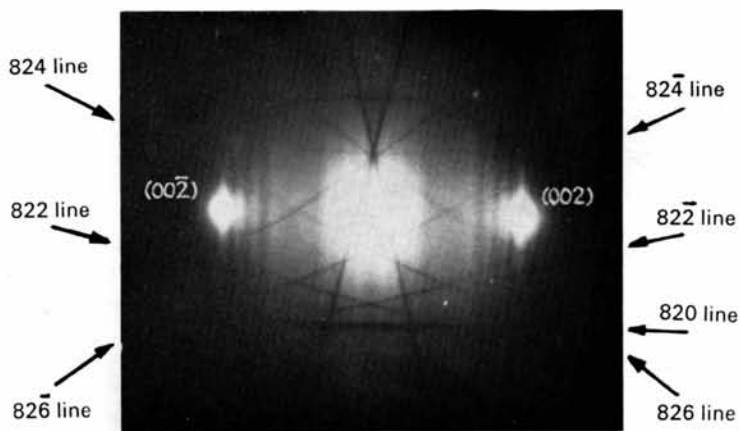


Fig.2. Transmission diffraction pattern showing fine structure oscillation, bending and doubling of Kikuchi lines, and displaced lines. Accelerating voltage, $E=80$ kV.

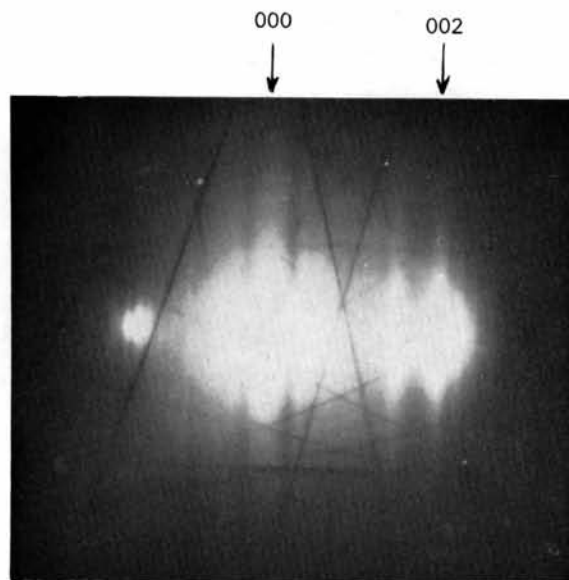


Fig.3. Diffraction pattern taken from the same crystal as shown in Fig.2, but the crystal was slightly tilted. $E=80\text{kV}$.

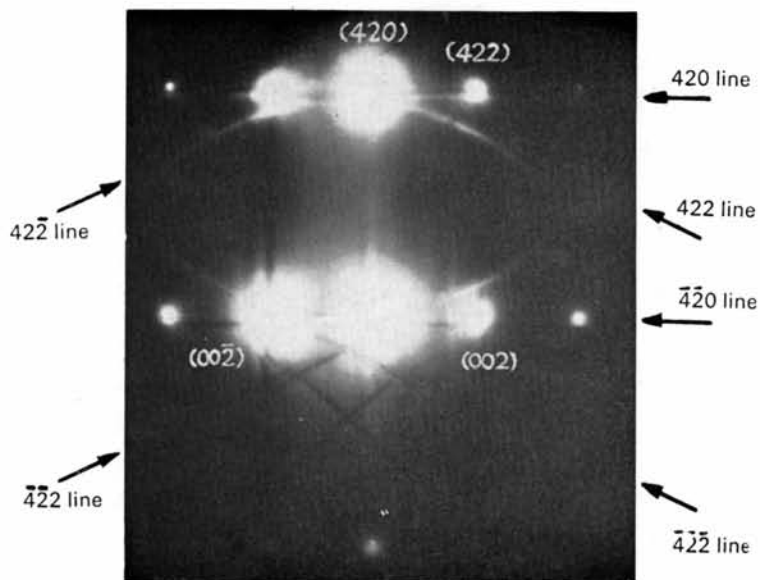


Fig.4. Diffraction pattern showing the contrast reversal of Kikuchi lines. $E=100\text{kV}$.

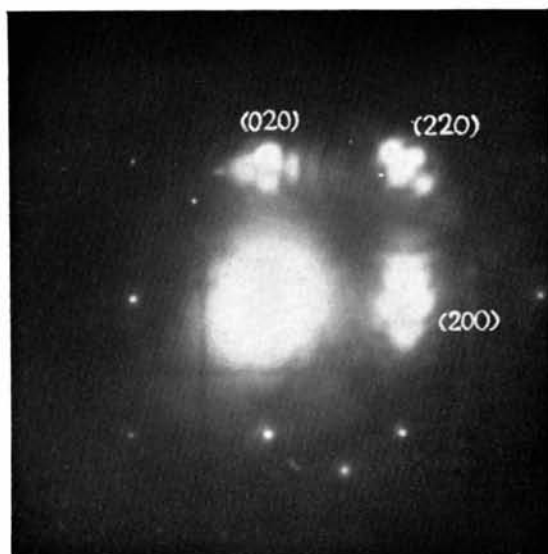


Fig. 5. Diffraction pattern showing a complicated diffuse scattering. Incident beam is almost parallel to the [001] axis. $E=80$ kV.

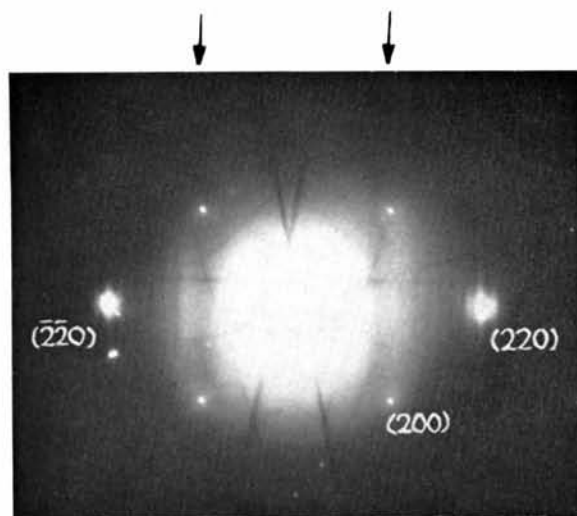


Fig. 6. Diffraction pattern showing asymmetrical lines bounding the 220 Kikuchi band. $E=80$ kV. Arrows show the 220 and $\bar{2}20$ line positions.

Fine structure

Fine structure effects in Kikuchi-line patterns were first reported by Uyeda, Fukano & Ichinokawa (1954) and explained qualitatively from Kainuma's theory (1955) of Kikuchi-line contrast. According to this theory, there is an oscillating thickness-dependent term,

$$\frac{-v^2}{8A_2^2} \frac{\sin 2A_2Z}{2A_2Z} \langle |f(\mathbf{s})|^2 \rangle.$$

Here, v is the Fourier potential of the reflexion, $4A_2^2 = \zeta_2^2 + 4v^2$, and ζ_2 the excitation error of the diffusely scattered wave.

The period of intensity oscillation in the fine structure may be explained from this oscillation term by assuming a suitable crystal thickness, as in the case of Uyeda *et al.* However, the amplitude of the oscillations calculated from such a term is very small, except for very thin crystals. Furthermore, the present observations, *viz.* the dependence of the fine structure on the reflexion condition of the incident beam and also the shift of the fine structure towards the direct or Bragg spot, suggest the fine structure to be related to the Bragg scattering of both the incident and the diffusely scattered waves. The most important oscillating term under these conditions is related to the term dominant in the expression for electron microscope contrast from diffuse scattering (Fujimoto & Kainuma, 1963; Fukuhara, 1963), *viz.*:

$$\frac{v^2(A^2 + A_1A_2)}{8A_1^2A_2^2} \frac{\sin(2A_1Z) - \sin(2A_2Z)}{2(A_1 - A_2)Z} \langle |f(\mathbf{s})|^2 \rangle,$$

where $4A^2 = \zeta_1^2 + 4v^2$, $4A^2 = \zeta_1\zeta_2 + 4v^2$ and ζ_1 is the excitation error of the incident wave. The oscillating factor in this expression is centred around $\zeta_1 = \zeta_2$, *i.e.* a line through the direct Bragg spot. Owing to the factor in front, the oscillations are, however, strongest on the side towards the Kikuchi line, and the qualitative behaviour of this expression was found to be in agreement with the observations outlined above.

A comparison of the experimental and calculated intensity curves for the fine structure has been made in the previous paper (Gjønnnes, 1966). Another case, where the excitation error for the Bragg spot is small, is shown in Fig. 7. The experimental curve is a photometer trace parallel to the 002 scattering vector from the pattern reproduced in Fig. 3. The calculation of the oscillating part was based on the form factor, $\langle |f(\mathbf{s})|^2 \rangle$, which was obtained so as to get consistency between the experimental background, *i.e.* assumed non-oscillating part, shown in the figure and the theoretical expression for the non-oscillating part. The calculations, which are based on a thickness of 1200 Å, are felt to account well for the observed magnitude of the fine structure oscillations. A somewhat better agreement of the background level was found to be obtainable when an independent background originating from, *e.g.* a supporting carbon film was subtracted from the curve. It should be pointed out, however,

that quantitative agreement was not reached when the excitation error, ζ_1 , was appreciably different from zero, the calculated fine structure being too weak.

According to the theory (Gjønnnes, 1966), the non-oscillating term has the following form,

$$\left(\frac{1}{2} + \frac{\zeta_1\zeta_2A^2}{8A_1^2A_2^2} \right) \langle |f(\mathbf{s})|^2 \rangle,$$

and the coefficient approaches a constant, $\frac{1}{2}$, when the excitation error of the incident beam tends to zero. We may mention that, when the Bragg condition is satisfied, the contrast of the Kikuchi line becomes very low and this agrees with the theoretical prediction. The weak or vanishing Kikuchi-line contrast when the incident beam is near a zone axis is also expected; in this case many beams are excited, and it seems reasonable that many different processes of the type (1) will tend to smear out the Kikuchi-line pattern.

Three- and four-beam interactions in the Kikuchi-line pattern

Three beam effects in the Kikuchi pattern have already been demonstrated by Shinohara (1932) who explained the excess envelope resulting when a set of deficient lines hkl , where l varies, crosses a pair of strong lines. Since then especially Pfister (1953) and Kambe (1957) have studied effects of three- and four-beam interactions on contrast and accurate position of the lines in Kikuchi and Kossel-Möllenstedt patterns. Here we shall discuss some of the details seen in the pattern of weak deficient $82l$ lines crossing the strong 002 pair in Fig. 2. [*cf.* Fig. 9(b)]. This geometry is very similar to that producing the Kikuchi envelope; the effects observed, notably the displaced lines mentioned above, can be related to the envelope. Since the features under discussion here do not show any fine structure and vary little with the direction of the incident beam, \mathbf{k}_0 , we shall neglect the Bragg scattering of the incident beam, which we take to lie inside the 002 pair, as in Fig. 2.

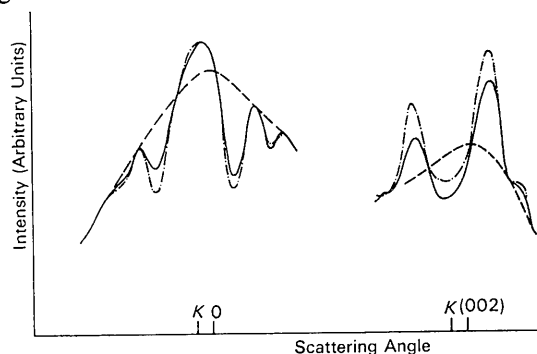


Fig. 7. Comparison between experimental and calculated fine structures of the 002 Kikuchi-line pair. Calculation was based on the direct beam excitation error $\zeta_1 = 0.5V_{200}$ and the crystal thickness of 1200 Å. Full line: experimental intensity curve. Broken line: assumed non-oscillating part. Dash-dot line: assumed non-oscillating part plus calculated oscillating part. K indicates Kikuchi-line positions. Positions of the direct spot and the 002 Bragg reflexion are also shown.

Let us designate positions on Fig. 2 inside the 002 pair by scattering vectors s and positions between these lines and the 004 lines by $s+h$, where h is the 002 reciprocal lattice vector, as shown in Fig. 8, where the point $s+g$ is at the excess Kikuchi envelope, g being one of the $82l$ reciprocal lattice vectors. Owing to the large reflecting power of the (002) planes, waves along k_0+s and k_0+s+h , or k_0+s-h , are strongly coupled. The main contribution to the contrast in the central $[s]$ region can be given by the ordinary deficient line intensity term, $|S(2)_{00}|^2 \langle |f(s)|^2 \rangle$, which has minima whenever the wave along k_0+s satisfies a Bragg condition. In the region between the 002 and 004 lines the main contribution to the diffuse intensity will be the 002 line excess term, $|S(2)_{h0}|^2 \langle |f(s)|^2 \rangle$. This term will have minima when a wave in the direction k_0+s+h satisfies a Bragg condition, which is at the Kikuchi-line position in this region, and also when the wave k_0+s satisfies a Bragg condition, which is at points on the displaced lines.

In order to determine the accurate position of the lines, we used the dispersion surface construction shown in Fig. 9(a), which corresponds to a section at the upper end of Fig. 9(b). The Fourier potentials of the reflexions $82l$ were assumed to be small, so that these reflexions could be regarded as perturbations on the ± 002 , 000 dispersion surface. Minima in $|S(2)_{00}|^2$ and $|S(2)_{h0}|^2$ then occur where the excitation errors $\zeta_{82l} = \zeta_j$, ζ_j being the 'anpassung' for a strongly excited branch of the unperturbed surface. The positions of the Kikuchi lines and displaced lines obtained in this way were found to agree well with the measurements on the plate. Solutions of the three- and four-beam equations along selected cross sections parallel to the 002 line were in qualitative agreement with the contrast effect observed. In particular, it was found that the calculated contrast, for example, of the 824 Kikuchi line is lower than the contrast of the $82\bar{2}$ and the displaced $822'$ and $82\bar{4}'$ lines, in the region between the 002 and 004 lines. This is in qualitative agreement with the observed pattern where the 824 line is missing in this region. By translating the $82l$ segments lying within the 002 lines through vectors, $g=82l$, as shown in Fig. 8, in order to obtain the corresponding parts of the excess lines, one can construct the excess envelope*. Extending this construction to segments outside the 002 pair, one also finds the general features of the excess contrast outside the envelope to be in accord with the observations of Shinohara (1932). In particular, the missing $82l$ segments between the 002 and 004 lines correspond to excess line segments systematically missing in Shinohara's patterns.

The reason for doubling of the 820 line within the 002 pair is not understood. Four-beam calculations of the contrast of this line did show, however, that a theoretical line profile is much broader inside the (002)

* The excess envelope cannot be seen on the plate, whereas part of a deficient envelope is visible below the 820 line.

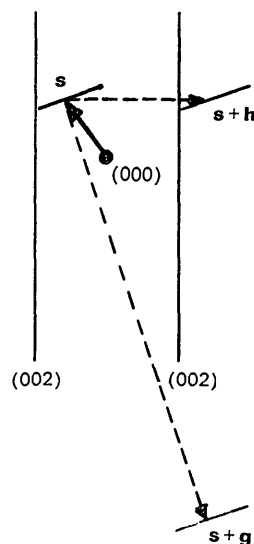


Fig. 8. Diagram showing relationship between points on a deficient line (s), a displaced line ($s+h$) and on the excess envelope ($s+g$); $h=002$, $g=82l$.

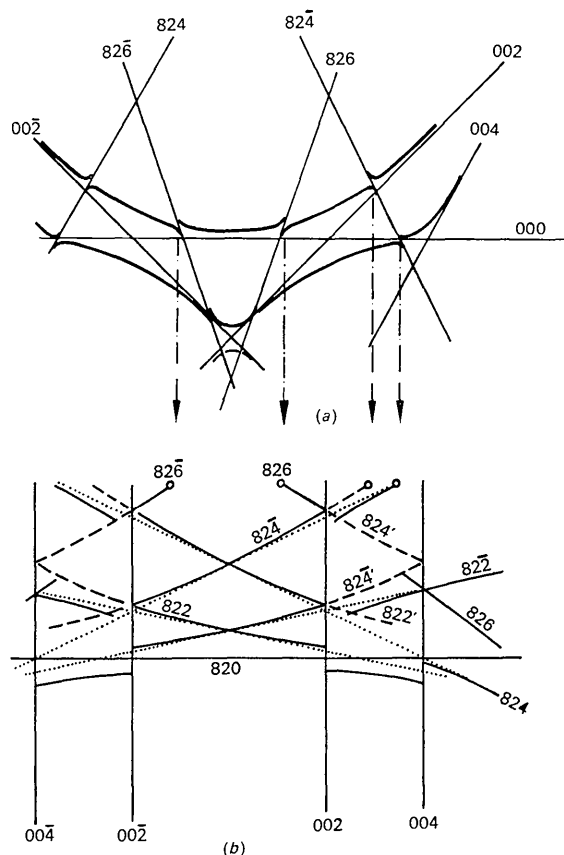


Fig. 9. (a) Dispersion surface construction for determination of Kikuchi-line and displaced-line positions. (b) Indexing of some of the lines in Fig. 2. Full line: Kikuchi lines. Broken line: displaced lines. Dotted line: Kikuchi-line positions expected from simple geometrical consideration of Kikuchi pattern.

pair than outside and calculated width inside the pair is nearly equal to the observed separation of the doublet.

Reversal of contrast along a Kikuchi line

The pattern reproduced in Fig. 4 includes in the $42l$ lines several of the features seen in the $82l$ line pattern discussed above. The excitation of some of the corresponding Bragg reflexions, particularly 420, leads, however, to fine structure effects and contrast changes. The most striking effect may be the change of contrast of the 422 and $4\bar{2}\bar{2}$ lines from excess to deficient on crossing the 420 line. The explanation for this reversal of contrast is illustrated in Fig. 10, where the incident beam is taken to satisfy exactly the 420 Bragg condition. Let us first consider a point, $\mathbf{s} + 00\bar{2}$, on the excess part of the $\bar{4}\bar{2}\bar{2}$ line. This point can be reached by several processes of the type given by equation (1). The two most important processes, $S(2)_{00\bar{2},420}S(1)_{420,000}f(\mathbf{s})$ and $S(2)_{00\bar{2},00\bar{2}}S(1)_{000,000}f(\mathbf{s} + 00\bar{2})$ are shown in the diagram. Of these, the former, which leads to an excess line, will dominate, because $|\mathbf{s}| < |\mathbf{s} + (00\bar{2})|$ and hence the diffuse scattering part $f(\mathbf{s})$ is the larger.

At the deficient part of the line, the situation is reversed, and of the two processes, $S(2)_{000,422}S(1)_{420,000}f(\mathbf{s}' + 00\bar{2})$ and $S(2)_{000,000}S(1)_{000,000}f(\mathbf{s}')$, the latter, which has the larger diffuse scattering amplitude, is a deficient term, leading to a deficient character of the line.

It may be mentioned that the reversal of contrast along the Kikuchi band observed by Shinohara & Matukawa (1933) and Pfister (1953) is a different effect, not related to the present phenomenon but to the absorption effect.

Asymmetrical lines bounding the Kikuchi band

The asymmetry of the lines described above (*General description of the patterns*) is of opposite sign to the asymmetry of the component lines in the excess Kiku-

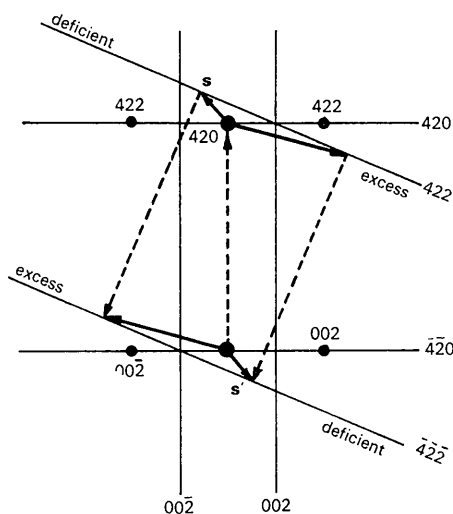


Fig. 10. Schematic illustration of Fig. 4, which shows reversal of Kikuchi-line contrast. Thick full lines and broken lines show the amplitude contributions mentioned in the text.

chi bands found from thin to moderately thick crystals by e.g. Pfister (1953) and in reflexion patterns by Miyake, Fujiwara & Suzuki (1962). Hence, it may be desirable to discuss briefly the different asymmetric contributions to the Kikuchi line, concentrating on the situation in Fig. 6, where the line pair is symmetrically disposed about the direct spot. The following expressions refer to the $\bar{\mathbf{h}}$ line*.

Kainuma (1955) derived the asymmetric term,

$$\frac{-2\zeta_2 v}{4A_2^2} \langle f(\mathbf{s})f^*(\mathbf{s} + \mathbf{h}) \rangle, \quad (2)$$

which is due to interference between the two scattering processes, $S(2)_{00}f(\mathbf{s})$ and $S(2)_{0h}f(\mathbf{s} + \mathbf{h})$. ζ_2 , the excitation error of the $\mathbf{k}_0 + \mathbf{s}$ wave, is negative inside the line pair. The form factor $\langle f(\mathbf{s})f^*(\mathbf{s} + \mathbf{h}) \rangle$ may have both signs. In a region around $\mathbf{s} = -\frac{1}{2}\mathbf{h}$ (roughly $\mathbf{s}(\mathbf{s} + \mathbf{h}) < 0$; Gjønnes, 1966) it will be negative for inelastic scattering, which we take to be the most important part of the diffuse scattering. Hence we expect the deficient part of the asymmetric line to be inside the line pair and the contrast to go to zero as the circle $\mathbf{s}(\mathbf{s} + \mathbf{h}) = 0$ is approached. This is in accordance with the observations in Fig. 6. Outside the circle $\mathbf{s}(\mathbf{s} + \mathbf{h}) = 0$ we might expect an asymmetric line of the opposite contrast; this will be weak, however, and has not been detected in the present experiments.

Pfister (1953) and Kainuma (1953) pointed out that anomalous absorption will lead to asymmetry in Kikuchi lines, and considered this to explain the change in sign of Kikuchi-band contrast with thickness. This asymmetry, which is a consequence of the well known asymmetry in the transmitted beam intensity, will have the same ζ_2 -dependence as the term given by equation (2). In the present case we found Lehmpfuhl & Molière's (1962) values of the anomalous absorption coefficient to give a contribution of about a third of the observed magnitude.

The third asymmetric contribution is a result of Bragg scattering of the incident beam; *viz.* interference between the two amplitude terms

$$S(2)_{00}S(1)_{00}f(\mathbf{s}) \quad \text{and} \quad S(2)_{0h}S(1)_{h0}f(\mathbf{s}).$$

This term has the form,

$$\frac{2\zeta_2 v}{4A_2^2} \frac{2\zeta_1 v}{4A_1^2} \langle |f(\mathbf{s})|^2 \rangle, \quad (3)$$

in the two-beam case (Gjønnes, 1966). When the direct spot is inside the line pair, this term is seen to lead to an asymmetrical contribution opposite in sign to the two former ones. For the ± 220 reflexions in Fig. 6, the excitation of the Bragg reflexions was found to be too weak to lead to any appreciable contribution. For reflexions with larger Fourier potentials relative to the excitation error in the symmetrical position, this term may be an appreciable contribution to Kikuchi bands with excess intensity inside the band, however.

* For the \mathbf{h} line, signs of \mathbf{h} should be changed throughout.

In the present case, we thus conclude that the term expressed by equation (2) gives the main contribution to the asymmetrical profile, and have compared the amplitude of this profile with the theoretical amplitude. The calculation of the form factor was based on one-electron form factors for the ions (Freeman, 1959, 1960) assuming the inelastic scattering in this region to be reasonably well described by one-electron scattering. The same comparison was made for the symmetrical line in the same position, obtained when the line pair was symmetrically disposed about the 220 Bragg reflexion. Results are given in Table 1.

Table 1. *Ratio of Kikuchi-line amplitude to background*

	Theoretical	Observed
Symmetrical line	0.5	0.4
Asymmetrical line	0.4	0.2-0.3

Owing to the uncertainties involved, especially in drawing the background, the comparison between experimental and theoretical values should be regarded as tentative only. Inclusion of anomalous absorption and other multiple diffuse scattering processes and thermal scattering does not seem warranted at this stage. The agreement in sign and magnitude indicates, however, that the term (2) gives the major contribution to the asymmetric profile in the present case.

Conclusion

The present study shows the theory of dynamical interactions in the diffuse scattering based on single diffuse scattering [equation (1)] to give an adequate explanation for most of the details in the patterns presented, although quantitative agreement was not always ob-

tained. Quite often it is essential to take Bragg scattering of the incident beam into account. Consideration of more than two beams is often required, as found by previous authors (Shinohara, 1932; Pfister, 1953; Kambe, 1957).

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