Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 500 words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible; and proofs will not generally be submitted to authors. Publication will be quicker if the contributions are without illustrations.

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The reflexion and transmission of X-rays near the Bragg angle in perfect absorbing crystals.

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Since Borrmann (1941, 1950) found that the absorption coefficient for Laue reflexion (i.e. reflexion of an X-ray beam passing through a crystal) is considerably smaller for angles near the Bragg angle, there have been several publications dealing with this anomalous transmission. The effect has been investigated experimentally with a two-crystal spectrometer and Geiger–Müller tube (Campbell, 1951*a*, *b*; Rogosa & Schwarz, 1952; Brogren & Adell, 1953). Campbell worked with a monochromator crystal at which the incident radiation underwent Bragg reflexion (i.e. the radiation was reflected at the surface of the crystal). Rogosa & Schwarz used a two-crystal spectrometer in the (1,1) position as monochromator, the emergent beam being directed on to a crystal where it underwent Laue reflexion.

The intensities of the transmitted and reflected radiation in the Laue case have been discussed by Zachariasen (1945, 1952), von Laue (1949, 1952), Ramachandran & Kartha (1952) and Hirsch (1952) among others. The last two plotted theoretical transmission and reflexion curves on the assumption that the incident radiation is monochromatic and parallel. There is a qualitative agreement between their results and experimental curves, but, since it is not experimentally possible to produce an X-ray beam exactly parallel and monochromatic, theoretical results hitherto obtained are not suitable for direct comparison with experimental results.

In connexion with an experimental investigation of anomalous transmission in calcite in the range 560–1930 X., we have carried out a theoretical calculation of the shapes of the transmission and reflexion curves for Laue diffraction. So far, the calculations are complete only for one wavelength–1537 X. (the Cu $K\alpha_1$ line). The experimental arrangement is illustrated in Fig. 1. The monochromator crystal A, a calcite crystal in the Bragg position with the surface parallel to the 211 plane, could be replaced by another crystal A' in which the 211 plane was perpendicular to the surface, giving reflexion in the Laue position. The analyser crystal was in all cases a calcite crystal in the Laue position. The intensities of the transmitted radiation T and the reflected radiation R were measured simultaneously with two Geiger–Müller tubes, which were carefully calibrated with respect to one another.

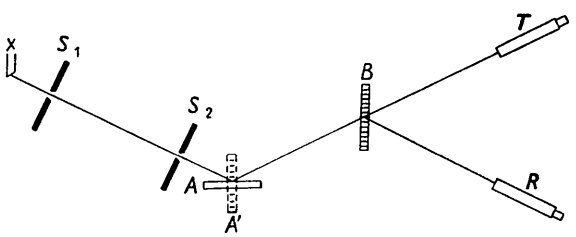

Fig. 1. The experimental arrangement. A is a monochromator crystal, cut for Bragg reflexion, which can be replaced by A', cut for symmetric Laue reflexion. The analyser crystal B, in which the anomalous transmission and reflexion were studied, is cut for symmetric Laue reflexion.

Let $R_B^n(\theta)$ and $R_B^p(\theta)$ denote the diffracted intensities for the reflected radiation in the Bragg case when the incident radiation is parallel and polarized (n and p denote the polarization directions of the two incident components), $R_L^n(\theta)$ and $R_L^p(\theta)$ the corresponding intensities in the Laue case, and $T_L^n(\theta)$, $T_L^p(\theta)$ the corresponding transmitted intensities in the Laue case. Then, for the two experimental arrangements used, and unpolarized incident radiation, we have

$$R(k) = \frac{\int_{-\infty}^{+\infty} R_B^n(\theta)\, R_L^n(\theta-k)\, d\theta + \int_{-\infty}^{+\infty} R_B^p(\theta)\, R_L^p(\theta-k)\, d\theta}{\int_{-\infty}^{+\infty} R_B^n(\theta)\, d\theta + \int_{-\infty}^{+\infty} R_B^p(\theta)\, d\theta}\,,$$

$$T(k) = \frac{\int_{-\infty}^{+\infty} R_B^n(\theta)\, T_L^n(\theta-k)\, d\theta + \int_{-\infty}^{+\infty} R_B^p(\theta)\, T_L^p(\theta-k)\, d\theta}{\int_{-\infty}^{+\infty} R_B^n(\theta)\, d\theta + \int_{-\infty}^{+\infty} R_B^p(\theta)\, d\theta}\,.$$

The integrated reflexion is $\int_{-\infty}^{+\infty} R(k)\, dk$

and the integrated transmission is $\int_{-\infty}^{+\infty} T(k)\, dk$.

For the Laue–Laue combination, R_B^n and R_B^p in the above equations are replaced by R_L^n and R_L^p.

The R and T functions in the respective cases may be derived from the dynamical theory for X-ray diffraction. $R(k)$ and $T(k)$ may then be computed by tedious graphical integrations. We will here content ourselves with an account of a comparison between the experimental and theoretical curves.

Both the experimental and theoretical curves are given in Figs. 2–4. Two series of measurements were made with the Bragg–Laue combination, the thickness of the Laue crystal being 0·047 and 0·034 cm. in the respective cases. The peak intensity obtained experimentally was in all cases lower than that calculated, but in order to facilitate comparison the ordinate scales were adjusted to give the

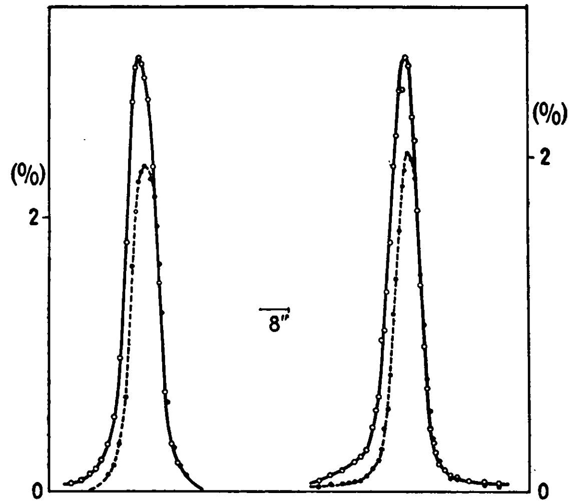

Fig. 2. Transmitted and reflected intensities of Cu $K\alpha_1$ radiation through a calcite crystal 0·47 mm. thick. Monochromator in Bragg position. The calculated values are plotted in the left-hand curve. Open circles in this and the following figures belong to the transmission curves. All intensities are given as a percentage of the incident intensity

two curves the same height. It will be seen that the curves agree remarkably well, apart from the fact that the experimental intensities are 10—25 % lower than the theoretical. The full width of the experimental R and T curves at half maximum intensity are in the main a few tenths of a second larger than those obtained by calculation, while the experimental values of the integrated reflexion and transmission are smaller than the theoretical. These differences seem to be due to slight imperfections in the crystals, and this is confirmed by observations made with two calcite crystals in the Bragg position in a two-crystal spectrometer. The general shapes of the corresponding curves exhibit a remarkable agreement. It is possible to draw some significant inferences from the curves. With the Bragg–Laue combination, the experimental R curves show the same asymmetry of the peak as that calculated, whereas the corresponding Laue–Laue curves are symmetrical. The calculations indicate that the Bragg diffraction pattern for an absorbing, perfect crystal is asymmetric, and this asymmetry is retained in the R curves for the Bragg–Laue combination. The asymmetry of the experimental curves thus confirms the dynamic theory as regards the Bragg pattern, a point which has not previously been demonstrated by experiment.

Comparison of the different measurements shows that the Laue–Laue arrangement is superior for this type of investigation. Since the full width for $R_L(\theta)$ at half maximum intensity is only about 2·8″, as against 7·4″

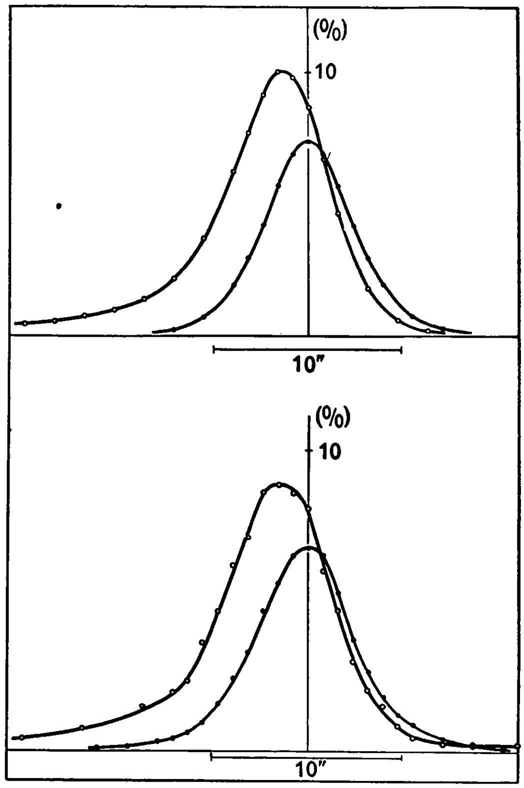

Fig. 4. Transmitted and reflected intensities of Cu $K\alpha_1$ radiation through a calcite crystal 0·34 mm. thick. Monochromator crystal in Laue position, 0·34 mm. thick. Upper curves give the theoretical values.

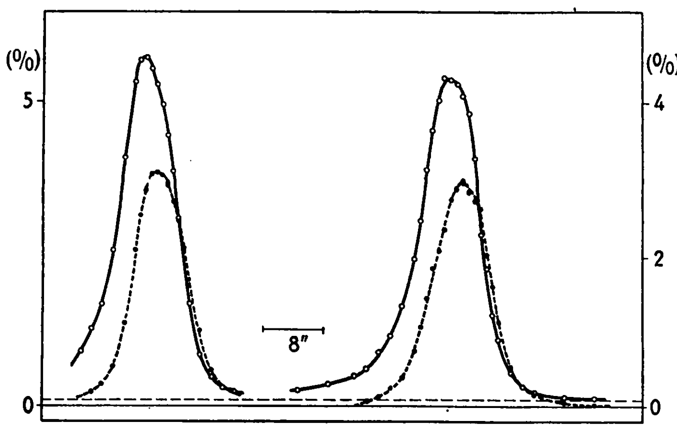

Fig. 3. Transmitted and reflected intensities of Cu $K\alpha_1$ radiation through a calcite crystal 0·34 mm. thick. Monochromator in Bragg position.

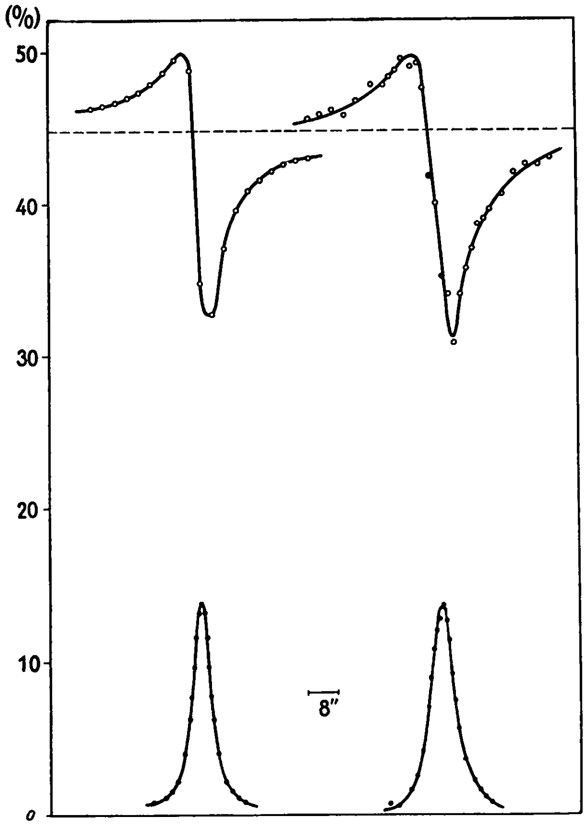

Fig. 5. Transmitted and reflected intensities of Mo $K\alpha_1$ radiation through a calcite crystal 0·34 mm. thick. Monochromator crystal in Laue position, 0·34 mm. thick. Calculated values plotted in the left-hand curves.

for $R_B(\theta)$, the broadening due to the angular width of the diffraction pattern is considerably smaller for the Laue–Laue combination

Calculations for other wavelengths are in progress, and Fig. 5 shows the experimental and theoretical results for the Laue–Laue arrangement and Mo $K\alpha_1$ radiation. The

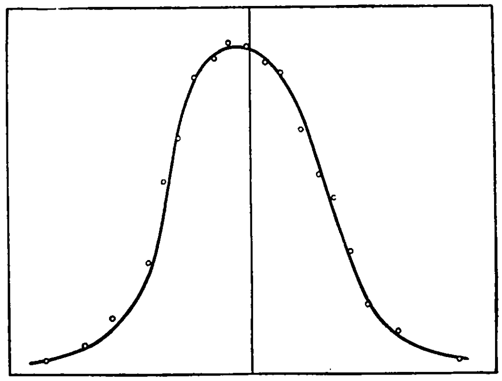

Fig. 6. The form of the reflexion curve in the Bragg–Laue combination for Cu $K\alpha_1$ radiation. Crystal thickness 0·47 mm. The curve gives the *calculated* form. The open circles are experimental values, which are adapted to the calculated values so that the same maximum is obtained.

agreement is good in this case as well. A full account of the investigation will be published later in *Arkiv för Fysik*.

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Sur une transformation martensitique de la phase protoxyde de fer.

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Dans un mémoire paru récemment dans *Acta Crystallographica* Willis & Rooksby (1953) ont étudié un changement de structure du protoxyde de fer à basse température. Nous voudrions signaler l'existence d'une transformation de type martensitique qui entraîne une autre modification du réseau de FeO.

Cette transformation se produit seulement dans les échantillons de protoxyde très riches en oxygène dont les paramètres, dans l'échelle absolue utilisée par Willis & Rooksby sont compris entre 4,280 et 4,283 Å environ. Elle se manifeste par un net élargissement des raies du protoxyde, sans qu'il soit possible de noter le dédoublement de certaines d'entre elles et de préciser ainsi le mode de déformation du réseau cristallin. On note, d'autre part, l'apparition d'un certain nombre de raies supplémentaires de faible intensité provenant d'un réseau quadratique d'arêtes $a = b = 6{,}11$ Å, $c = 8{,}32$ Å.

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