

Short Communications

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The 'two-beam' pattern in electron diffraction. By P. GOODMAN, *Division of Chemical Physics, C.S.I.R.O., Chemical Research Laboratories, Melbourne, Australia*

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Results of three calculations are presented, chosen to illustrate the continuance of weak beam interaction at very great crystal thicknesses. The calculations are idealized in that they ignore the diffuse and inelastic intensities, and furthermore consider only systematic interactions.

Recently in response to a discussion n -beam calculations were run to very large thicknesses using the multi-slice method (Cowley & Moodie, 1967). The 'two-beam' pattern, commonly obtained from thick crystals, was formerly sometimes held as evidence that the two-beam dynamic condition could be approached by increasing crystal thickness. However, these observations relate to anomalous transmission of the strongly excited and zero beam which occurs in the presence of weak-beam interactions. The continuance of these interactions is illustrated in principle by these calculations.

In Fig. 1, for a non-absorbing MgO structure considering $\{h00\}$ systematic interactions, the closest weak beams are shown to oscillate with unchanging relative importance. Introducing structure-dependent absorption ($V_{200}^i = 0.14$ volt *etc.*; Goodman & Lehmpfuhl, 1967) causes the strong beams to approach non-oscillating values while the weak beams continue in importance although oscillating. More precisely, the transmitted main beams have lower absorption ($\mu_0 - \Delta\mu$) than mean value μ_0 (anomalous transmission), and the damping of the weak beam oscillations is approximately the *reduced* value ($\mu_0 - \Delta\mu$), since the ratio (I mean weak beam)/(I mean main beam) is almost constant at large

thickness. This is found for two models, *viz.* V_h^i constant or $\propto V_h$, though for the former model this ratio is larger. The point at which the strong beams become non-oscillating is roughly dependent on the V_h^i magnitudes, for one model. The amplitude of the weak beam oscillation relative to that of the main beams continues to increase with thickness (Fig. 2).

These curves should not be compared with experiment since they ignore diffuse and inelastic scattering. Simple consideration of inelastic scattering will show that the associated diffuse beams exhibit greater anomalous transmission than the two sharp beams, so that these latter gradually transfer their energy to two diffuse regions. The weak beams are similarly diffused but their relatively low intensity and the strong diffuse background may make their observation difficult.

Thus the practical end-point might be said to resemble the two-beam ($V_h + iV_h^i$) theory end-point when the latter has lost its oscillations. Even this conclusion is subject to the assumption of a perfect crystal. In practice imperfections such as stacking faults, inclusions *etc.* may occur in thick crystals. Fig. 3 shows the result of introducing a break in the crystal at a certain thickness. Such an imperfection is seen to have a large effect on the weak beam intensities;

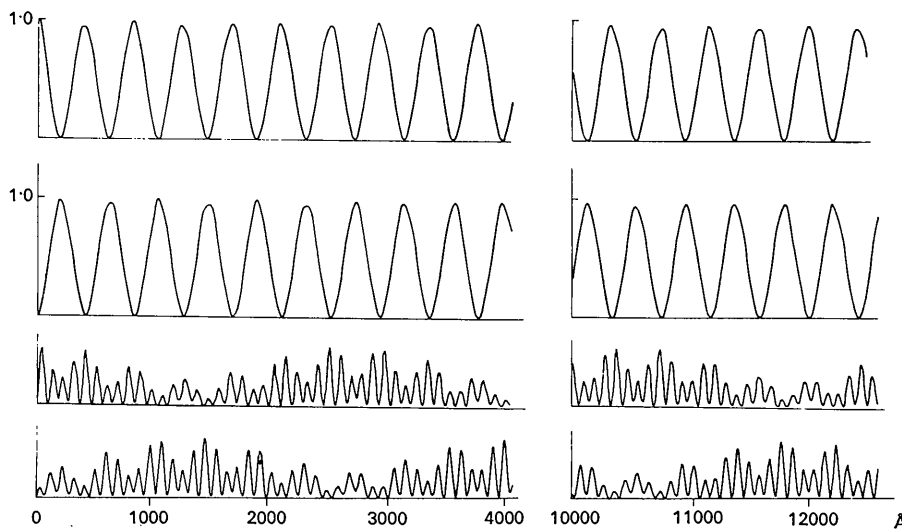


Fig. 1. Intensities calculated for the 000, 002, 400 and $00\bar{2}$ reflexions of MgO for $\{h00\}$ systematic interactions using 13 beams, with $\zeta_{002} = 0$, and $V_h^i = 0$. Intensity scale for weak beams (lower two curves) is $20\times$ that for the strong beams.

immediately after the break these are greatly increased. The results are contrasted to those for a perfect crystal, added to the diagram. Firstly the strong beams acquire an increased high frequency component from weak-beam interaction. This effect is characteristically produced by localized defects, and could also be observed as fine fringes in the

convergent beam patterns. Secondly the anomalous transmission of the strong beams and the relationship existing between the strong and weak beams of Fig.2, has been destroyed. The former might be expected from the theory of anomalous transmission. Although a gross defect was used for this illustration, very small deviations from peri-

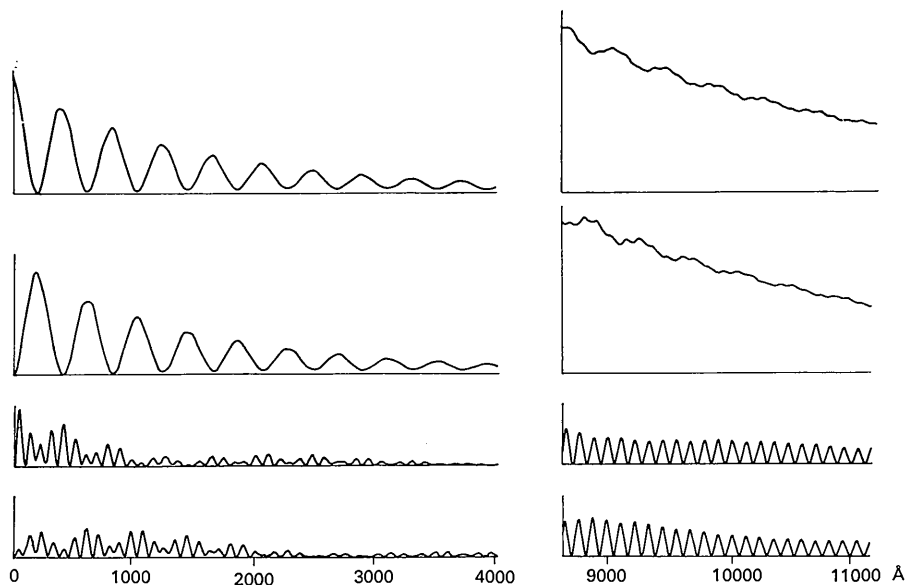


Fig.2. Calculation as for Fig.1, with $V_h^t = 0.014$ volt. The relative scale between the beams is as in Fig.1, with a further intensity magnification of 100 for the right hand sections.

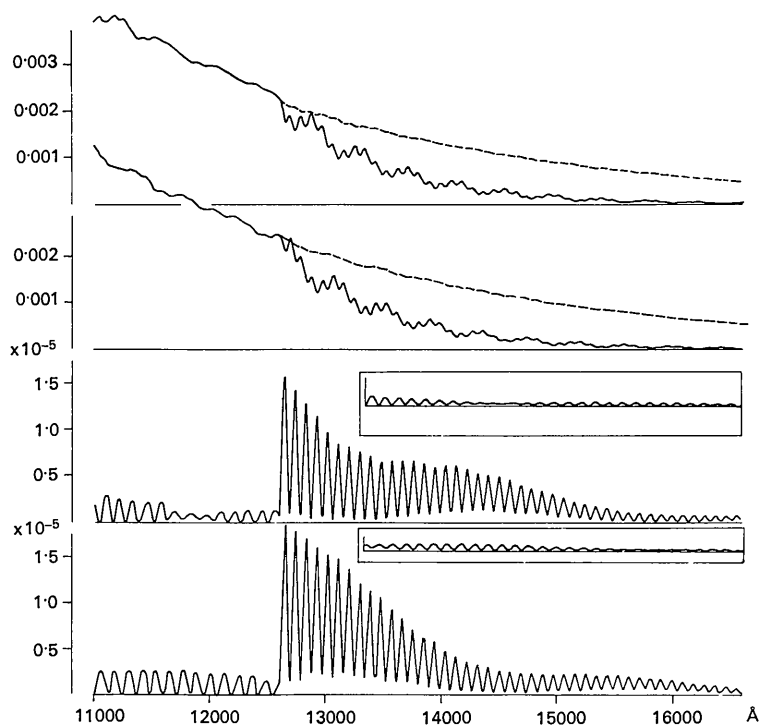


Fig.3. Calculation repeated with a break of 100 \AA introduced into the crystal at 12600 \AA . For comparison, result from the perfect crystal (calculation of Fig.2) is inserted by broken curve (strong beams) and inset curve (weak beams). Intensity scale is $400 \times$ that of Fig.1.

odicity act to increase the relative importance of the weak beams so that the condition of two strong beams may never be reached.

Excellent examples of thick-crystal patterns have been given by Uyeda & Nonoyama (1966*a, b*) showing the conditions of two diffuse regions. Furthermore they found that anomalous transmission did not occur in thick specimens which contained high dislocation densities. More realistic calculations take into account the non-systematic interactions, which themselves introduce absorption (Gjønnes, 1962). Without additional absorption processes these effects can partially reverse at another thickness as pointed out by Hall & Hirsch (1965). However in general, and for example particularly near a high-order zone axis (*e.g.* Fig. 10, Goodman & Lehmpfuhl, 1968) a total damping is produced, *i.e.* the energy never returns to the central beam. The intensity remaining distributed between the weak beams

is therefore relatively more significant than in the systematic case. A detailed investigation of this problem for different structures has recently been concluded by Fisher (1968).

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Thermal expansion of strontium sulphide, SrS and strontium chloride, SrCl₂. By A. A. KHAN* and V. T. DESHPANDE, *Physics Department, College of Science, Osmania University, Hyderabad-7, India*

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Accurate values of the lattice constants of SrS and SrCl₂ have been determined at different temperatures in the ranges 30–273°C and 26–294°C respectively. The coefficients of lattice thermal expansion, obtained from these data, could be expressed by:

$$\begin{aligned} \text{SrS} : \alpha_t &= 9.26 \times 10^{-6} + 3.36 \times 10^{-8}t + 1.11 \times 10^{-12}t^2 \\ \text{SrCl}_2 : \alpha_t &= 20.80 \times 10^{-6} + 11.29 \times 10^{-9}t + 46.60 \times 10^{-12}t^2, \end{aligned}$$

where α_t is the coefficient of thermal expansion at $t^\circ\text{C}$.

Lack of experimental data in the literature on the thermal expansion of strontium sulphide (SrS) and strontium chloride (SrCl₂), led the authors to undertake a study of the temperature variation of the lattice constants and the coefficients of thermal expansion of these crystals. Conventional methods, involving the use of (i) X-ray back-reflexion powder photography, (ii) least-squares treatment of the film data and (iii) statistical analysis of the results, were employed to obtain precision values of the lattice constants at different temperatures along with estimates of the limits of errors (Deshpande & Mudholker, 1960; Deshpande & Khan, 1963; Jette & Foote, 1935).

SrS (NaCl type) was studied at seven different temperatures between 30° and 273°C. Strontium chloride, which is usually obtained in the hydrated form (SrCl₂·6H₂O, trigonal), had to be heated at 300°C for about three hours to give the anhydrous powder (cubic, CaF₂ type). This powder was packed in the specimen holder of the camera and kept well protected from atmospheric moisture during exposures. Pictures were taken at eleven different temperatures between 26° and 294°C.

Table 1. *Values of the lattice constants of SrS and SrCl₂ at different temperatures*

SrS		SrCl ₂	
Temperature °C	<i>a</i>	Temperature °C	<i>a</i>
30	6.0233 ± 0.0004 Å	26	6.9792 ± 0.0005 Å
62	6.0249	54	6.9833

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Table 1 (cont.)

SrS		SrCl ₂	
Temperature °C	<i>a</i>	Temperature °C	<i>a</i>
92	6.0273	74	6.9868
129	6.0302	87	6.9896
159	6.0326	112	6.9933
230	6.0395	130	6.9956
273	6.0440	164	7.0019
		217	7.0098
		246	7.0158
		273	7.0203
		294	7.0241

Table 1 gives the values of the lattice constants of the two crystals at different temperatures along with the estimated accuracies. The coefficients of thermal expansion were obtained by the method suggested by Deshpande & Mudholker (1961) and could be expressed as follows:

$$\begin{aligned} \text{SrS} : \alpha_t &= 9.26 \times 10^{-6} + 3.36 \times 10^{-8}t + 1.11 \times 10^{-12}t^2 \\ \text{SrCl}_2 : \alpha_t &= 20.80 \times 10^{-6} + 11.29 \times 10^{-9}t + 46.60 \times 10^{-12}t^2. \end{aligned}$$

Here α_t is the coefficient of thermal expansion at $t^\circ\text{C}$.

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