

oscillating function of thickness, and sensitive to any averaging of phase. The problem of contrast arising from a

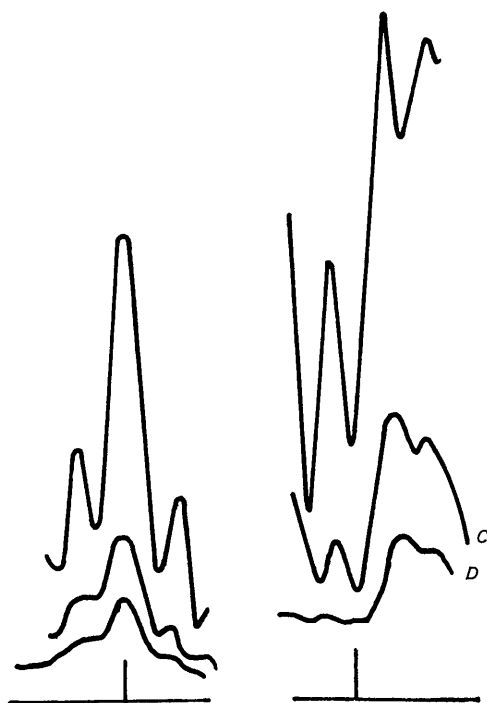


Fig. 3. Microphotometer curves from the MoS_2 pattern, from the 110 and 000 beams. From top to bottom the scans are, inside the convergent beam aperture, inelastic pattern close (C) and distant (D) from the aperture.

* The terms Kossel and Kikuchi are used in their usual sense: Kossel lines are formed by an external convergent or divergent source; Kikuchi lines are produced by scattering sources within the crystal.

strong structure factor, outside the angular range of incidence, is complicated and requires individual consideration, but the result is not necessarily identical to that predicted by classical Kikuchi* line theory which involves an integration over the Z coordinate (*i.e.* averaging of a different kind).

Patterns from MoS_2 [Fig. 1(c), (d)] with the 110 reflexion excited show, besides extended contrast as above, strong absorption asymmetries in the background. Asymmetry associated with the 110 background (Fig. 3) can come only from inelastic scattering from sources localized within the crystal (*e.g.* core excitations). It is also noteworthy that the fringe detail arises in the low angle scattering, and the asymmetry arises in the high-angle scattering (compare C and D in Fig. 3). Asymmetry of the 000 beam is high, and at 50kV, exceeds that of the elastic pattern. This shows the influence of the 'accidental' lines. As seen in the underexposed pattern of Fig. 1(c) these lines cause increased asymmetry from dynamic interference, and this influence is diffused in the background scattering and so is always involved in the background intensity. This emphasizes the difficulties associated with interpreting absorption asymmetries from bent crystals in the electron microscope, where these lines are not resolved.

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Formation of rhombohedral polytypes of cadmium iodide. By V. K. AGRAWAL, *Department of Physics, Hastinapur College, New Delhi-21, India*

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Theoretical stacking-fault energies of all known rhombohedral structures of cadmium iodide have been calculated. It has been found that the polytypes occurring more frequently do not possess minimum energies. It can be explained only if mixed dislocations of Burgers vectors ($c + a/3 + 2b/3$) are considered responsible for the creation of rhombohedral polytypes in cadmium iodide.

Out of nearly 160 polytypes of CdI_2 reported so far (Trigunayat & Chadha, 1971), fourteen possess rhombohedral structures. The complete structures of only 7 of them, $12R$, $24R$, $30R$, $36R$, $42R$, $60R$ and $72R$, have been determined. Their formations can be thought of as resulting from the common structure $4H$, due to the occurrence of a mixed dislocation made up of a screw dislocation of Burgers vector $(n/3)c$ along the c axis and an edge dislocation of Burgers vector $(a/3 + 2b/3)$ in the basal plane. The structure of a crystal is affected by the Burgers vector of the

screw dislocation alone. When it is an integral multiple of the height of the unit cell of the basic structure $4H$, the resulting structure will evidently belong to a polytypic rhombohedral series $[(22)_n 13]_3$. On the other hand, a screw dislocation of Burgers vector $(2n+1)c/2$, which is a non-integral multiple of the height of the basic unit cell, will give rise to another polytypic series $[(22)_n 1212]_3$. Since the former type of screw dislocations has the layers in perfect fit with each other in contrast to the latter type which produces a misfit, the former should occur more frequently

Table 1. *Stacking fault energies*

Polytype	Zhdanov symbol	Theoretical stacking fault energy*
12R	[13] ₃	$E_a = 2E_2 + E_3 + 4E_4 + 3E_5 + 4E_6 + 4E_7 + 8E_8 + \text{---}$
24R	[2213] ₃	$E_b = 2E_2 + E_3 + 4E_4 + 2E_5 + 5E_6 + 3E_7 + 8E_8 + \text{---}$
30R	[221212] ₃	$E_c = 2E_2 + 4E_4 + 2E_5 + 6E_6 + 2E_7 + 7E_8 + \text{---}$
36R	[22112121] ₃	$E_d = 2E_2 + 4E_4 + 2E_5 + 6E_6 + 3E_7 + 7E_8 + \text{---}$
42R	[(22) ₂ 1212] ₃	$E_e = 2E_2 + 4E_4 + 2E_5 + 6E_6 + 2E_7 + 7E_8 + \text{---}$
60R	[(22) ₃ 1223] ₃	$E_f = 2E_2 + 4E_4 + 2E_5 + 6E_6 + E_7 + 8E_8 + \text{---}$
72R	[(22) ₄ 1223] ₃	$E_g = 2E_2 + 4E_4 + 2E_5 + 6E_6 + E_7 + 8E_8 + \text{---}$

* The fault energy is represented by the number of pairs of separation N which are not in proper stacking sequence compared to the common structure sequence multiplied by the distortional energy E_N per pair. They present $(n/3) H \rightarrow nR$ transformation energy per $\frac{1}{3}$ of the unit cell of nR type.

than the latter. This implies a great abundance of polytypes of the former series, which agrees fully with experimental observations. The known members of series [(22)_n 13]₃ are the types 12R and 24R and of the other series [(22)_n 1212]₃, 30R and 42R. Of 12R and 24R, the former occurs more abundantly than the latter because the energy required for the creation of mixed dislocations generating 12R and 24R, as proportional to the square of their Burgers vector whose magnitudes are $[c^2 + \frac{1}{3}a^2]^{1/2}$ and $[(2c)^2 + \frac{1}{3}a^2]^{1/2}$, respectively, is evidently less for the former than the latter. This also explains the rare occurrence of higher polytypes which otherwise, on the stacking fault energy considerations alone (Table 1), should occur very frequently. The polytype 36R can be explained in terms of a mixed dislocation of Burgers vector $(2c' + a/3 + 2b/3)$ where $c' = 3c/2$. The formation of 60R and 72R can be understood by considering the cooperation of two screw dislocations of the same hand along with a partial edge dislocation. For any nR polytype, since every $n/3$ th layer is part of the same spiral surface extending throughout the crystal, any stacking fault once generated in a layer will expand along the appropriate spiral surface to the $n/3$ th, $2n/3$ th, n th, \dots , neighbouring layer, thereby causing a periodic repeated slip.

The rhombohedral structures are found to occur almost on the upper face of the crystals. This is significant in the

sense that the screw dislocations are generated towards the later stages of the growth as the high energy required for their creation can be available from the crystal only when it has grown to a considerable volume whereas edge dislocations may be created at any stage of the growth.

Recently Prasad & Srivastava (1971) have calculated theoretical stacking fault energies of 60R, 72R, and 32H and have shown that it is minimum for the proposed structures and consequently a new possible method of determining atomic structures has been suggested. But, from stacking fault energy considerations alone, it is found that rhombohedral polytypes should possess the structures [(22)_n 13]₃, not the proposed structures. Therefore, the stacking fault energy criterion alone is of limited value in determining the atomic structures of polytypes.

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Thermal expansion of strontium molybdate By V. T. DESHPANDE and S. V. SURYANARAYANA, *Physics Department, College of Science, Osmania University, Hyderabad-7, India*

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A precise X-ray determination of the lattice parameters of strontium molybdate (SrMoO_4) has been made in the temperature range 26 to 658°C. Using these data the coefficients of the lattice thermal expansion, α_a and α_c , along and perpendicular to the tetragonal axis respectively, have been evaluated. The temperature dependence of these coefficients could be expressed in the following forms: $\alpha_a = 6.58 \times 10^{-6} + 10.62 \times 10^{-9}t - 1.25 \times 10^{-12}t^2$ °C⁻¹, $\alpha_c = 16.43 \times 10^{-6} + 20.26 \times 10^{-9}t - 8.16 \times 10^{-12}t^2$ °C⁻¹. Here t is the temperature in degrees Celsius.

Recently we have studied the temperature variation of the lattice parameters and the principal coefficients of thermal expansion of a number of scheelite type compounds. The data obtained on some of the compounds have already been published [KIO_4 (Deshpande, Pawar & Suryanarayana, 1967); NaIO_4 (Deshpande, Suryanarayana & Pawar, 1968); CaMoO_4 (Deshpande & Suryanarayana, 1969a); CdMoO_4

(Deshpande & Suryanarayana, 1969b); SrWO_4 (Deshpande & Suryanarayana, 1969c) and BaWO_4 (Deshpande & Suryanarayana, 1970)]. The present note reports similar results obtained on strontium molybdate, SrMoO_4 . No published work on either the macroscopic expansion or the lattice expansion measurements on this solid, is available in the literature.