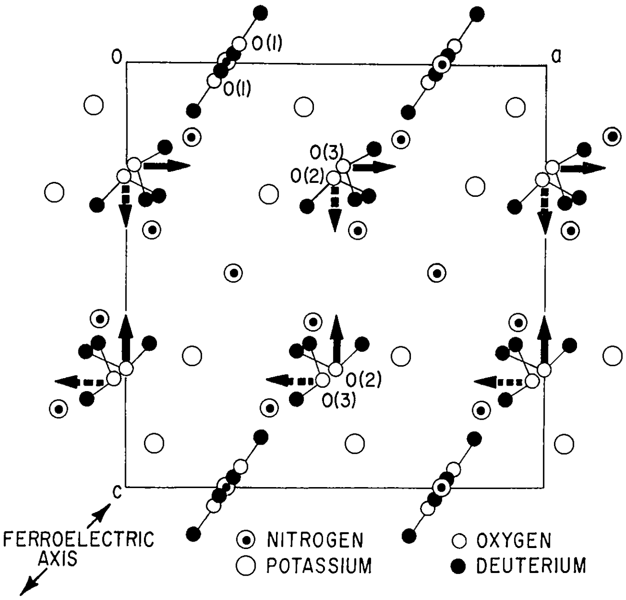

Fig. 6. KFCT water molecule layer at $y=0{\cdot}5$ showing the ferroelectric axis. Water dipoles associated with one ferroelectric state are marked by the solid arrows, and with the other state by dotted arrows.

Further elucidation of the complex behavior of KFCT below the Curie temperature can best be obtained by a series of neutron diffraction studies at lower temperatures with an electrical field first along [$\bar{1}$01] and then a reversed field. This type of investigation was made by Bacon & Pease (1955) on KH_2PO_4 and would also allow a check on possible movements of the K^+ and the ferrocyanide ions.

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Short Communications

Contributions intended for publication under this heading should be expressly so marked; they should not exceed about 1000 *words; they should be forwarded in the usual way to the appropriate Co-editor; they will be published as speedily as possible. Publication will be quicker if the contributions are without illustrations.*

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Arcing and polytypism.

By V. K. Agrawal, *Department of Physics, Hastinapur College (University of Delhi), Moti Bagh, New Delhi-23, India*

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An X-ray study of the arcing phenomenon in polytypic crystals of CdI_2, PbI_2 and $CdBr_2$ has revealed that various polytypes are formed by the creation of stacking faults at different regular intervals during crystal growth.

An X-ray study of a large number of crystals of three polytypic substances, *viz.* 120 of CdI_2 (Agrawal & Trigunayat, 1969*a,b*), 60 of PbI_2 (Agrawal, Chadha & Trigunayat, 1970*a*) and 12 of $CdBr_2$ (Agrawal & Trigunayat, 1970), has revealed that the arcing phenomenon, which consists of an extension of the diffraction spots into small arcs or closed rings on X-ray Laue photographs, is interrelated with the phenomenon of polytypism. The arcing phenomenon has been satisfactorily explained in terms of edge dislocations created during crystal growth (Agrawal & Trigunayat, 1969*a*,*b*), whereas to explain the polytypism, various theories (Verma & Krishna, 1966) have been put forward. The only theories which have received good experimental recognition so far are the dislocation theory (Frank, 1951) and the disorder theory (Jagodzinski, 1954) but these, too, could not explain the formation of all the polytypes discovered so far. An attempt has therefore been made to explain the phenomenon. Apart from the academic and mineralogical interests involved, this phenomenon has evoked more material interest in recent years as it has been found that the different polytypes of a substance may possess different semiconducting properties. Knippenberg (1963) has found a correlation between the structure type and the band gap for SiC.

The relation between the phenomena of arcing and polytypism (being inferred from the following experimental observations), suggests that the edge dislocations which originate the arcing phenomenon are also responsible for the formation of polytypes. The experimental observations establishing the correlation between arcing and polytypism are as follows:

(*a*) The arcing phenomenon occurs in nearly 42% of CdI_2 crystals, whereas in PbI_2 crystals its occurrence is limited to only about 5%. The occurrence of polytypes, other than the common types (2*H* in PbI_2 and 4*H* in CdI_2), in PbI_2 crystals is also less frequent in comparison with CdI_2 crystals. Only 10% of PbI_2 crystals occur as such polytypes, whereas for CdI_2 crystals the proportion is nearly 25%. This shows that the frequency of generation of edge dislocations, which is governed by the stacking fault energy, is lower in PbI_2 than in CdI_2. The experimental observation of lesser incidence of streaking in PbI_2 substantiates this conclusion.

(*b*) The upper and lower parts of a crystal, as picked up from a crystallizing dish, have always been found to display different degrees of arcing and usually the lower part shows more arcing than the upper one. A similar effect is observed for polytypism. The upper and lower parts of a crystal are generally found to be different polytypes, occurring in syntactic coalescence with each other, and the lower part is usually either a higher polytype or is more disordered than the upper part. The basic cause for both these observations is to be attributed to the non-uniform rate of generation of dislocations during growth. The edge dislocations occur at a fast rate during the initial stages of growth, when the high saturation makes the crystal grow rapidly. Since the force required to move a dislocacation is much lower than that to create it, the dislocations can move freely inside the crystal during growth. The movement of partial edge dislocations of Burgers vector $\mathbf{a}/3\ \langle 10\bar{1}0\rangle$ on the basal planes causes complete layer displacements, creating stacking faults, whereas the movement of unit edge dislocations of Burgers vector $\mathbf{a}/3\ \langle 11\bar{2}0\rangle$ on the basal planes will not affect the layer sequence in the structure. If the stacking faults are stabilized by vibration entropy (Jagodzinski, 1954), a high polytype (higher than 2*H* or 4*H*) is formed, otherwise a disorder polytype is obtained. The arrangement of the edge dislocations into tilt boundaries which have large angles on account of the fast occurrence of the former, results in the observed large arcing. However, if a high polytype succeeds in forming, the arcing is far less, the reason for which is described in the following paragraph. Towards the later stages, the growth conditions become well-stabilized, thus greatly reducing the chances of creation of the edge dislocations and the stacking faults. Hence, the upper part of the crystal is usually the lower polytype and is relatively free from arcing.

(*c*) The arcing is usually found to occur in the crystals of common polytypes. Only a few higher polytypes have shown arcing or rings on their Laue photographs; even in these the sizes of the rings or the arcs are small. The underlying reason is that a part of the energy available for the creation of dislocations during growth is utilized in creating stacking faults by complete layer displacements.

(*d*) A few crystals of CdI_2 show arcs consisting of two or more spots which belong to different polytypes occurring on the same part of the crystals. The arcing is due to the formation of boundaries of partial dislocations which divide the crystal into a number of blocks. The dislocations are created at different intervals in different portions of the crystal, giving rise to different sequences of layers in them. Thus, various polytypes are generated in different portions of the crystal.

These observations clearly point to a correlation between the phenomena of arcing and polytypism. A substance with a greater degree of polytypism should necessarily show more arcing, too. However the reserve may not be true because the formation of polytypes requires the stabilization of stacking faults, *i.e.* the occurrence of

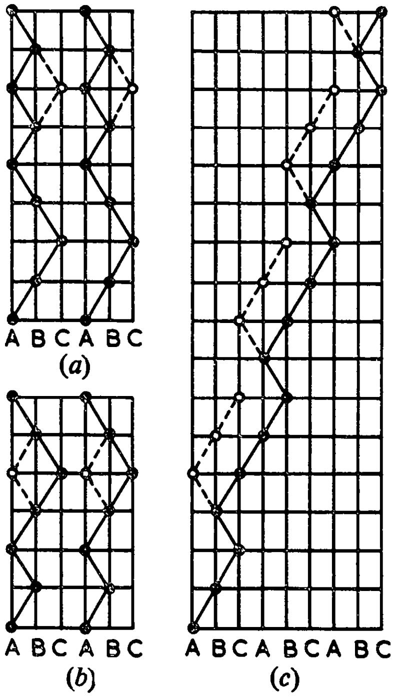

Fig. 1. The unit-layer stacking in CdI_2 or PbI_2 structure containing a single fault (*c*) and a double fault [(*a*) and (*b*)]. The horizontal lines are the sections of the unit-layers. (*a*), (*b*) and (*c*) represent a CdI_2 polytype 8*H* having the Zhdanov symbol $[(22)_{n=1}1111]$, a PbI_2 polytype 6*H* having the Zhdanov symbol $[(11)_{n=1}22]$ and a CdI_2 polytype 12*R* having the Zhdanov symbol $[(22)_{n=0}13]_3$, respectively. Open circles and broken lines indicate the zigzag characteristics to the common structure.

the layer displacements at some definite regular intervals, which may not always be possible, as in the case of $CdBr_2$ crystals. It is seen that these crystals always display large arcing and heavy streaking on their X-ray photographs (Agrawal & Trigunayat, 1970), indicating that the edge dislocations and the stacking faults occur more frequently in them than in CdI_2 or PbI_2 crystals. The frequency of layer displacements may be too high to render the chances of their stabilization a remote possibility. Hence, the observed low incidence of polytypism in $CdBr_2$ crystals is accounted for.

These observations lead to the conclusion that various polytypes are formed by the creation of stacking faults at different regular intervals. The formation of several polytypes of CdI_2, *e.g.* $30R$, $42R$, $8H_b$, $24H_g$ (Chadha & Trigunayat, 1967*a,b*), $12R$ (Agrawal & Trigunayat, 1968), $20H_p$, $20H_q$ (Agrawal, Chadha & Trigunayat, 1970*b*), $18H_g$, $30H_f$, $24R$ and $36R$ (Jain, Chadha & Trigunayat, 1970) and of PbI_2 (Agrawal *et al.*, 1970*a*) have already been explained in similar terms. Recently Mardix, Kálmán & Steinberger (1968) have also explained the formation of various polytypes of ZnS in terms of periodic slip at regular intervals. The formation of various structural series, *viz.* $(22)_n1111$ in CdI_2 (Agrawal *et al.*, 1970*b*) and $(11)_n22$ in PbI_2 (Agrawal *et al.*, 1970*a*) can be easily explained by considering a double stacking fault occurring in their common polytypes at regular intervals of $4(n+1)$ layers and $2(n+2)$ layers, respectively [Fig. 1(*a*),(*b*)]. The common polytypes of CdI_2 and PbI_2 are the types $4H$ and $2H$, respectively. A double fault is formed when a single fault is immediately followed by another single fault [Fig. 1(*a*),(*b*)]. The formation of rhombohedral polytypes of CdI_2 belonging to the $[(22)_n13]_3$ series, *viz.* $12R$ (Agrawal & Trigunayat, 1968) and $24R$ (Jain *et al.*, 1970), can be easily explained in terms of a single stacking fault occurring at an interval of $4(n+1)$ layers in the common type $4H$ [Fig. 1(*c*)]. CdI_2 polytypes belonging to $(22)_n11$ series (Chadha & Trigunayat, 1968) can be explained by considering an intrinsic fault (a low energy type fault which does not disturb nearest-neighbour packing), produced by shearing operations on the $\{0001\}$ planes about the B layer, in the common type $4H$ with layer sequence $(A\gamma B)(C\alpha B)$ after every $(4n+2)$ layers.

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A comment on the paper *Coherent crystal radiation affects the measurement of the X-ray linewidths* (Das Gupta & Welch, 1968)

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(*Received* 11 *March* 1969 *and in revised form* 26 *January* 1970)

Das Gupta & Welch have introduced the concept of 'coherent crystal radiation' to explain their experiments. As a consequence of their interpretation the fundamental X-ray line widths taken with the double-crystal spectrometer are in error. As shown in the present paper, the results of Das Gupta & Welch can be explained by means of the existing theories of the double-crystal spectrometer and triple-crystal diffractometer.

In their recent paper Das Gupta & Welch (1968) have made essentially two statements:

(I) In the double crystal spectrometer arrangement (DCS) the second crystal is the source of a 'coherent crystal radiation' (CCR) (which results in the appearance of extra peaks in the triple-crystal diffractometer (TCD) rocking curves).

(II) As a consequence of (I) DCS is 'obviously unsuitable to determine the fundamental widths of X-ray emission lines'.

The aim of the present paper is to show that one can explain both the extra peaks and the line-widths by means of the existing theories of DCS (Compton & Allisson,

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