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A comment on Prasad and Srivastava's paper *On the occurrence of Zhdanov numbers* 1, 2 *and* 3 *in the zigzag sequence of cadmium iodide polytypes.*

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As a comment on the paper by Prasad & Srivastava [*Acta Cryst.* (1972). A28, 494–497] it is shown that the possibility of occurrence of CdI_2 polytypes having Zhdanov numbers higher than 3 in zigzag sequence cannot be ruled out theoretically for their structure determination.

Recently Prasad & Srivastava (1972) have analysed the genesis of CdI_2 polytypes in the light of transposition mechanism and have shown that possible Zhdanov numbers are limited to 1, 2 and 3. It was demonstrated that the Cd/I glide led to *ABC* sequences which were energetically unfavourable. However in the present study it is found that there are many known polytypes (an example is given below) which can be explained only if the Cd/I glide is also considered along with the I/I glide, although the Cd/I glide is less probable in comparison with the I/I glide because of the different binding forces between Cd/I and I–I layers. In addition, the sandwiches I–Cd–I remain unsheared in the process of I/I glide.

Consider two units of the common type 4*H* having *ABC* sequence $(A\gamma B)(C\alpha B)$ to explain the formation of an 8*H* type (221111), already discovered by Mitchell (1956). It can be explained by introducing two successive single faults, known as a double fault (Agrawal, 1970), created through I/I and Cd/I glide, respectively. On glide along an I–I glide plane a stacking fault of the type $(A\gamma B)(C\alpha B)(A\gamma B)\downarrow(A\beta C)$ results; further, glide along the Cd–I or I–Cd glide plane generates a fault of the type $(A\gamma B)(C\alpha B)(A\gamma B)(A\beta\downarrow B)$ or $(A\gamma B)(C\alpha B)\,A\gamma B)\,(A\downarrow\alpha B)$; the arrow indicates the position of the glide plane. However, a synchro-shear motion (Amelinckx, 1964) takes place to bring the Cd atoms from tetrahedral interstices (β or α positions) again into octahedral sites (γ positions). Thus two coupled partial dislocations of opposite sign and the same Burgers vector in the adjacent lattice planes are required to produce this structure. There are many other identified polytypes, *viz.* 8*H* (121121), $12H_1$ (22221111), $12H_2$ (22211211), $12H_3$ (11123211), $12H_4$ (21211212), *etc.* which cannot be explained without taking the Cd/I glide into consideration.

The formation of all the identified structures can be explained by considering screw dislocations or by introducing growth faults and/or deformation faults like single and double faults in the basic structure 4*H*. If a polytype has a Zhdanov number higher than 3, triple, quadruple and higher faults are required to explain its formation. But their occurrence is less probable than single and double faults because of energy considerations. However, the creation and subsequently the occurrence of polytypes having Zhdanov numbers higher than 3 cannot be ruled out theoretically.

The terms double fault and triple fault, used in the quoted paper, are in fact equivalent to two and three single faults, respectively, occurring at an interval of one sandwich. It had led to some confusion as the authors had obtained the same *ABC* sequence *ABACABCBABAC*... (sequences viii and xii of their paper) by introducing two different types of faults, a double fault and a single fault, respectively, in the basic 4*H* structure.

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Refinement of merohedrally twinned crystals.

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A simple procedure is outlined whereby merohedrally twinned crystals may be refined with existing least-squares programs. It is applicable to crystals containing any number of twin individuals and can handle different twin laws simultaneously.

The general problem of structure refinement of merohedrally twinned crystals has been discussed by Grainger (1969) and Sudarsanan, Young & Donnay (1973). The methods proposed by these authors have certain disadvantages. The summed intensity method of Grainger reduces the number of reflexions in the refinement, and the method outlined by Sudarsanan *et al.* requires extensive manual manipulation

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