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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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and does not give a full-matrix solution in the strictest sense. Here, a simple procedure is outlined whereby twin data may be refined by inclusion of the volume fraction in the normal equations, using least-squares programs that are generally available.

If $[x_i]$ are the positional coordinates of one part of the twin and the twinning operation is represented by the matrix $[T_{ij}]$, the coordinates of the twinned fraction of the crystal (with reference to the axes of the untwinned fraction) are given by

$$[x_i'] = [T_{ij}][x_i].$$

Similarly, the anisotropic temperature factors β'_{ij} of the twinned fraction are given by

$$\beta'_{ij} = \sum_{k=1}^{3}\sum_{l=1}^{3}[T_{ik}][T_{jl}]\beta_{ij}.$$

The above equations are used to generate the parameters of the twinned fraction for each twin law and are subsequently applied as linear constraints in the refinement cycles. If n is the number of atoms in the asymmetric unit and p is the number of twinned fractions, the site occupancies (s) of one twin-equivalent atom in $p-1$ fractions are refined with the following constraints operative

$$s_{ij} = s_{1j} \qquad i=2,n;\ j=1,p-1$$
$$s_{ip} = 1 - \sum_{j=1}^{p-1} s_{1j} \qquad i=1,n.$$

No manual manipulation is required once the refinement is in progress. All reflexions are used and there is only one additional variable per twin law. Several least-squares programs (*RFINE*: Finger, 1968; *CRYLSQ*: Stewart, Kruger, Ammon, Dickinson & Hall, 1972) are currently available that incorporate linear constraints of the necessary form.

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International Union of Crystallography

Commission on Crystallographic Apparatus

Abstracts of Papers for the Madrid Conference on Anomalous Scattering

The Inter-Congress Conference on Anomalous Scattering, organized by the Commission on Crystallographic Apparatus, was held 22–26 April 1974 in Madrid, Spain for the purpose of stimulating new and current use of anomalous scattering and for improving the present theoretical and experimental approaches to the interpretation and measurement of anomalous scattering. Invited papers were presented in the following sessions: 1. Theoretical calculation of dispersion corrections. 2. Experimental determination of dispersion corrections. 3. Absolute intensity measurement including anomalous scattering. 4. Effects of dispersion on atomic parameters. 5. Use of anomalous scattering in protein structure analysis. 7. Absolute configuration and tensorial properties. 8. Novel methods for using anomalous scattering.

Abstracts of 35 papers have been printed and are available, price £1 postaid, from the Executive Secretary International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England.

The proceedings of the Conference will be published in book form at a date to be announced later.

Book Reviews

Works intended for notice in this column should be sent direct to the Book-Review Editor (M. M. Woolfson, Physics Department, University of York, Heslington, York YO1 5DD, England). As far as practicable books will be reviewed in a country different from that of publication.

The dynamics of atoms in crystals. By W. COCHRAN. Pp. 145, Figs. 85. London: Arnold, 1973. Price £4.60; (paperback) £2.30.

As Professor Cochran points out in an excellent introductory chapter, the study of the vibrations of atoms in crystals has a long history, the initial papers being published more than 60 years ago. However, the number of papers on this subject remained quite small until the late 1950's, and the enormous volume of literature existing today has been published only in recent years. The aim of Professor Cochran's monograph is to expound as simply as possible the basic principles of the subject and to guide the student, by means of selected references for further reading, through the morass of published material.

The topics covered in the first five chapters are real and reciprocal-space lattices, dynamics of one-dimensional chains, simple three-dimensional crystals, interatomic force constants, the determination of phonon frequencies, particularly by means of neutron coherent inelastic scattering, and the interpretation of these data in terms of force models for various solids. Following this introduction to the basic concept of harmonic phonons, there are chapters on various related physical properties such as heat capacity, thermal conductivity, dielectric and optical properties (infrared absorption, Raman and Brillouin scattering) and thermal ex-