TEACHING AND EDUCATION IN CRYSTALLOGRAPHY

This is a new section in the *Journal of Applied Crystallography*, to which authors are encouraged to submit contributions describing any aspect of the teaching of crystallography. Submitted papers in this section can take the form of short communications, teaching notes or even full research publications. Potential authors are invited to send their contributions to any member of the Editorial Board.

J. Appl. Cryst. (1995). **28**, 223

Three-dimensional periodicity and inversion axes in crystals.

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(*Received* 7 *July* 1994; *accepted* 2 *September* 1994)

Abstract

One of the basic tenets of the 'lattice' is the strict adherence to 1-, 2-, 3-, 4- or 6-fold symmetry. The proof is simple and found in most crystallography text-books. However, proofs for inversion axes, which are distinct from rotation axes, are not available. The following presentation is not necessarily unique but may be unfamiliar to crystallographers and so is offered here as part of the new section on *Teaching and Education in Crystallography*.

Crystal lattice

We start with the explicit requirement that crystals are represented by a three-dimensional 'LATTICE' with periodicity in all respects. Thus we have lattice vectors that are transformed by various symmetry operations. The lattice vector is given by

$$\mathbf{r} = l_1\mathbf{a}_1 + l_2\mathbf{a}_2 + l_3\mathbf{a}_3,$$

with the usual meanings for each symbol. l_1, l_2, l_3 are integers.

For the present discussion, we focus on the following symmetry elements: (i) rotation axes; (ii) inversion axes; (iii) roto-reflection axes. There has been no attempt to prove restrictions for the inversion and/or roto-reflection axes prior to the original work of Sharma (1983). A general statement about the square matrix is in order. The trace of similar square matrices is the same (Margnau & Murphy, 1956). It was this point that was raised by my daughter that led to the original work (Sharma, 1983).

Rotation axes in crystals, C_n, n

The transformation matrix in an orthogonal system of coordinates is, where α is the angle of rotation,

$$\begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The trace is $2\cos\alpha + 1 =$ an integer (positive, zero or negative). Hence, the permitted values of α are 360, 180, 120, 90 and 60°, corresponding to C_1(1-fold), C_2 (2-fold), C_3 (3-fold), C_4 (4-fold) and C_6 (6-fold) rotation axes and none other. This is a simple and elegant proof and takes into account the three-dimensional nature of crystals.

Inversion axes, $\bar{n}$

The transformation matrix now is

$$\begin{pmatrix} -\cos\alpha & \sin\alpha & 0 \\ -\sin\alpha & -\cos\alpha & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

the trace is $-2\cos\alpha - 1 =$ an integer (positive, zero or negative), and once again the allowed values of α are 360, 180, 120, 90 and 60°. Hence, the inversion axes are restricted to $\bar{1}$, $\bar{2}$, $\bar{3}$, $\bar{4}$ and $\bar{6}$ and no other.

Roto-reflection axes, S_n

Again, the transformation matrix has the form

$$\begin{pmatrix} \cos\alpha & -\sin\alpha & 0 \\ \sin\alpha & \cos\alpha & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

and the trace is $2\cos - 1 =$ an integer (positive, zero or negative). The inevitable conclusion drawn above requires that S_1, S_2, S_3, S_4 and S_6 axes are the only ones compatible with a three-dimensional periodic lattice.

A discussion of the relationship between inversion axes and the roto-reflection axes is presented by Sharma (1982) from a teaching point of view.

The author gratefully acknowledges the enthusiasm of his daughters, N. V. Sharma-Bowman and Renuka D. Sharma when helping them in problems in mathematics arising out of their days as students. The author is also indebted to the referee for constructive criticism and suggestions.

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