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CRYSTALLOGRAPHY

1970

SovietRxiv

Abstract

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UDC 548.736

CRYSTALLOGRAPHY

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SELECTION OF THE BASIC SYSTEM FROM A VECTOR SYSTEM BY A PEAK OF MULTIPLICITY TWO (FEDOROV GROUP $P\bar{1}$)

The algorithm for selecting the basic system (b.s.) from a vector system (v.s.) by a peak of multiplicity two for the general case of an acentric crystal was proposed in ([1]). Below we consider the case of a centrosymmetric crystal (Fedorov group $P\bar{1}$).

Let the centrosymmetric b.s. consist of N points (Fig. 1, $N = 6$), forming $N_1 = N/2$ pairs; then in the corresponding v.s. all points will be connected into $N_1(N_1 - 1)/2$ parallelograms, and the maximum multiplicity of a v.s. peak will be equal to 2 (a peak at the midpoint of a side of a parallelogram)* (Fig. 2).

Fig. 1. B.s. of 6 points. Fedorov group $P\bar{1}$

We choose as the initial one in the v.s. any peak located at the midpoint of a side of some parallelogram, for example r_{13}(I). The system of points selected by vector I is shown in Fig. 3.

In comparison with ([1]), at this stage only 2 copies of the b.s. points** are selected, related by the inversion point at the midpoint of vector I, and vector r_{13} will be common to these two copies. At the second stage of selection, for vector II we choose an as yet unused, likewise double, peak at the midpoint of another side of the parallelogram (Fig. 2), and carry out a shift along it among the points already selected by vector I. The system of points recorded in Fig. 4 will be the desired one.

Fig. 2. V.s. corresponding to the b.s. of Fig. 1. Vectors I and II, I′ and II′ are selected

It is not difficult to see that any of the parallelograms found in the v.s. in the process of its decoding may be taken as the initial parallelogram. The two stages of selection by vectors I′ and II′ (Fig. 2, Fig. 3b) lead to the same b.s.

* The case is considered in which in the independent part of the b.s. there are no pairs of points n_1 and n_2, m_1 and m_2 with $r_{m_1 m_2} = r_{n_1 n_2}$, since, by virtue of the centrosymmetry of the basic system, two more pairs $\bar{m}_1$ and $\bar{m}_2$, $\bar{n}_1$ and

$\bar{n}_2$ must necessarily arise in it, and thus in the v.s. there will be a peak of multiplicity 4.

** By virtue of the centrosymmetry of the b.s.

Fig. 3. Result of developing the v.s. along vector I (a) and vector I′ (b)

In matrix form, the notation according to ([2]) for the o.s. of Fig. 1 gives the vector system in the form

$$\begin{array}{cccccc} 11 & 12 & 13 & 14 & 15 & 16 \\ 12 & 22 & 23 & 24 & 25 & 26 \\ 13 & 23 & 33 & 34 & 35 & 36 \\ 14 & 24 & 34 & 44 & 45 & 46 \\ 15 & 25 & 35 & 45 & 55 & 56 \\ 16 & 26 & 36 & 46 & 56 & 66 \end{array} \qquad (1)$$

When selecting along vector I, four copies of ([1]) are simply pairwise equal (marked by the rectangle and oblique hatching)

$$\begin{array}{cccccc} 11 & 12 & 13 & 14 & 15 & 16 \\ 12 & 22 & 23 & 24 & 25 & 26 \\ 13 & 23 & 33 & 34 & 35 & 36 \\ 14 & 24 & 34 & 44 & 45 & 46 \\ 15 & 25 & 35 & 45 & 55 & 56 \\ 16 & 26 & 36 & 46 & 56 & 66 \end{array} \qquad (2)$$

and as a result only two systems are selected,

$$\begin{array}{cccccc} 11 & 12 & 13 & 14 & 15 & 16 \\ 22 & 23 & 24 & 21 & 25 & 26 \end{array} \quad (= 64 \quad 54 \quad 44 \quad 34 \quad 24 \quad 14 \text{ from } ([1])) \qquad (3)$$

with common points $11 = 22$ and $13 = 24$.

Fig. 4. O.s. selected along vectors I and II (I′ and II′)

Similarly to the way this was done in ([1]), when selecting from the v.s. along vector II, the following appear:

$$\begin{array}{cccccc} 11 & 12 & 13 & 14 & 15 & 16 \\ 31 & 32 & 33 & 34 & 35 & 36 \end{array} \quad (= 64 \quad 54 \quad 44 \quad 34 \quad 24 \quad 14 \text{ from } ([1])), \qquad (4)$$

$$31 \quad 32 \quad 33 \quad 34 \quad 35 \quad 36 \quad (= 62 \quad 52 \quad 42 \quad 32 \quad 22 \quad 12 \text{ from } ([1])),$$

A successive shift of the v.s. by vector I and then by II, in matrix notation, reduces to the superposition of pairs (3) and (4), after which only one system of points remains, 11 12 13 14 15 16, which is the desired one.

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Received
16 III 1970

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2. M. Burger, *Crystal Structure and Vector Space*, IL, 1961.

Note: Figure translations are in progress. See original paper for figures.