$$g_0(x) = f(x)$$
$$g_1(x) = 2f(x) - f(x) * h(x)$$
$$\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots$$
$$g_{n+1}(x) = g_n(x) + [f(x) - g_n(x) * h(x)] . \quad (30)$$

Iteration stops when the correction term, $f(x) - g_n(x) * h(x)$, is of the same order of magnitude as the errors in the original data.

For solving the more general equation (24), the convolution operation in (30) is replaced by the integral of (24).

The fully sharpened version of the data of Fig. 2 is shown in Fig. 8. The first equatorial halo is not plotted as it will of course have zero azimuthal spread. There is marked agreement with the crystalline fibre pattern.

7. Conclusions

The azimuthal sharpening technique described in this paper is particularly applicable where a well separated equatorial halo is available for determining the distribution of entity axes. In principle, a meridional halo would be even easier to use since it gives a section of the distribution directly. However, meridional reflexions are much more sensitive to disorder such as curved chains or lack of longitudinal register between the chains which will smear the reflexion along the layer line. This component of smearing would be difficult to remove.

The smearing process of § 5 could, in fact, be carried out in a single step for any form of $\Phi(\alpha_1, \alpha_2)$, although this would involve complicated double integrals. Thus the iterative method could be used to reverse the process in a single step. However, this requires knowledge of $\Phi(\alpha_1, \alpha_2)$ rather than its projection. For fibre symmetry, we would additionally need to solve (12) for Φ_2.

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Theoretical Approach to the Derivation of Condensed Models of Crystal Structures Based on Square-Type Layers

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Condensed models of crystal structures based on the stacking of equal square-type layers corresponding to the three possible symmetries (plane groups *p4m*, *p4g* and *p4*) are studied in a general way for the regular stacking modes. The minimum set of standard sheets required to represent any structure based on each layer symmetry is derived by considering transparent sheets, either square or standard rectangular in shape. In the latter case four sheets are necessary for *p4m* and *p4g* patterns, and eight sheets for *p4* patterns. An example of a *p4g* layer occurring in the $CuAl_2$ and TlSe structures is presented.

Introduction

The representation of crystal structures, which is a three-dimensional problem, can in most cases be formally decomposed into a $2D+1D$ (two-plus-one-dimensional) problem by considering sections of the structure (layers) and the way they stack together. Crystal-structure models can therefore be designed by slicing the structure into layers of atoms and drawing them on transparent sheets which are then mounted one above another with a proper spacing. Such models are particularly useful for representing inorganic close-packed structures and are called 'condensed models' (Lima-de-Faria, 1965, 1966). Standard sheets have been designed where the packing atoms are represented by full circles, and all the possible interstitial sites resulting from the stacking of the adjacent close-packed layer are drawn as dashed circles. Any layer of a close-packed structure is figured out simply by painting in the occupied interstitial sites, and in this way a versatile sys-

tem is available from which a wide range of crystal-structure models can be made.

The minimum set of standard rectangular sheets necessary to build any layer sequence involving the regular modes of stacking has already been derived for the square close-packed layers [parallel to (001) of the cubic closest packing] and for the closest-packed layers (Figueiredo & Lima-de-Faria, 1972, 1977). It was then shown that a determining factor is the location of the layer pattern in relation to the centre of the sheet.

A theoretical approach to the representation of crystal structures by condensed models is presented by considering the symmetry of the layer pattern in connexion with the stacking modes for equal layers and the shape of the sheet. This general treatment is illustrated through the consideration of layers with square symmetry (plane groups *p*4*m*, *p*4*g* and *p*4).

General remarks

The origin of the unit cell of the layer pattern is the reference position of the layer, denoted *A* (Fig. 1, top left). Points α and β (midway along the unit-cell edges) and point *B* (unit-cell centre) are the projections of the points homologous to *A* in following layers, stacked on the first layer according to the regular modes. The layer positions related by the projected stacking vectors **A**α and **A**β (translations $0,\frac{1}{2}$ and $\frac{1}{2},0$ respectively) correspond to the mode of stacking symbolized by the letter *b*; vector **AB** (translation $\frac{1}{2},\frac{1}{2}$) corresponds to the stacking mode denoted by the letter *f*, and the stacking without translation of the layer pattern is symbolized *s* (Lima-de-Faria & Figueiredo, 1976).

In the representation of crystal structures by condensed models, the rigid-body translation of a layer, which corresponds to a certain stacking vector, is achieved by an appropriate rotation of the layer pattern suitably drawn on a transparent sheet. As the two faces of the sheet are indistinguishable, even rotations which reverse the face are allowed.

The process of generating different stacking positions of the layers with the same transparent sheet involves the use of rotations coplanar with or perpendicular to the plane of the sheet. The rotation of the sheet must generate a new position differing from the starting position only by a translation, a condition imposed by the definition of the stacking modes. If the layer pattern has mirror lines, the rotation of the sheet about diad axes parallel to these lines will reproduce the layer pattern, but displaced in relation to the initial position, thus satisfying the stacking condition men-

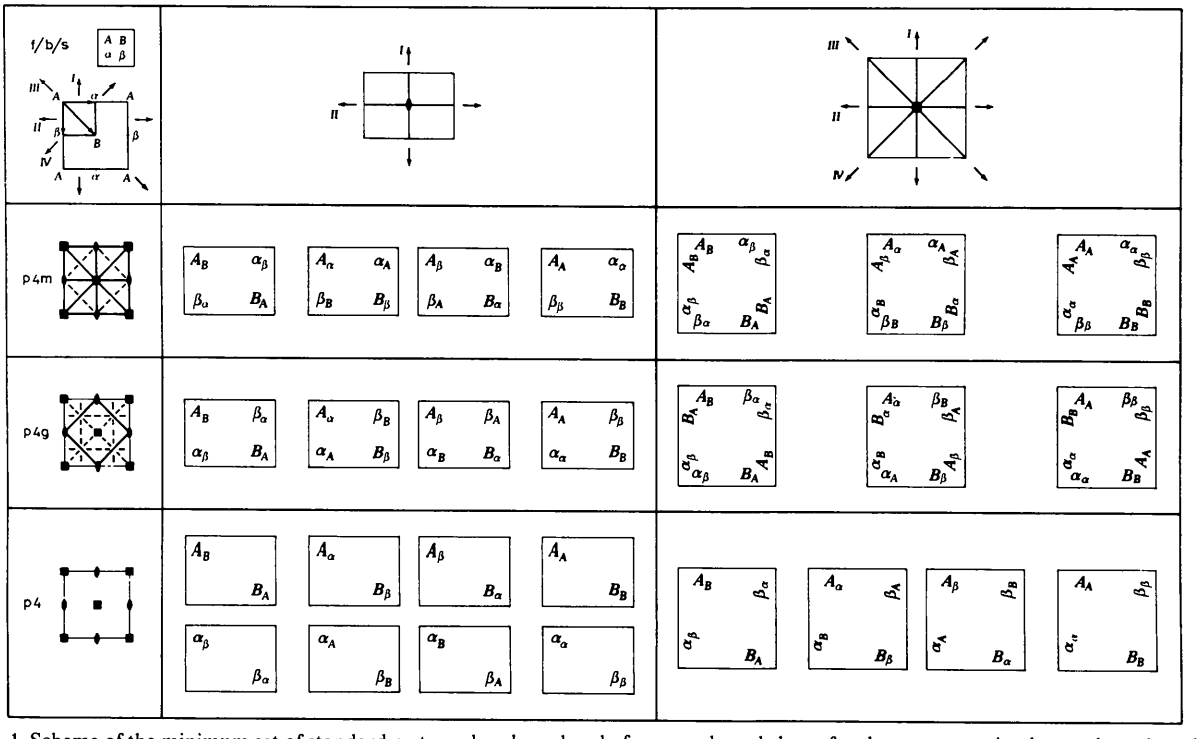

Fig. 1. Scheme of the minimum set of standard rectangular-shaped and of square-shaped sheets for the representation by condensed models of structures based on square-type layers stacked in any possible sequence of the regular stacking modes. The position projection net, the projected stacking vectors and the choice of the sheet centre, defined by the diad axes coplanar with the sheet, are represented in the first column, which contains also the possible symmetries of the layer pattern. The useful symmetry operators of the rectangular and of the square transparent sheets are represented at the top of the figure. The standard sheets are aligned in columns according to the various stacking modes: *f*, *b* and *s*.

tioned above. The same holds for the glide lines, but, because of the translation inherent in the glide reflexion, the rotation axes of the sheet may even coincide with such lines. Moreover, if the stacking vector has its origin over a useful symmetry element of the layer pattern, the corresponding rotation axis of the sheet will contain the middle point of the stacking vector.

To generate a maximum number of different stacking positions by appropriate rotations of one sheet, the location of the sheet centre in relation to the symmetry elements of the layer pattern has to be such as to maximize the number of symmetry elements which can be useful.

In the case of square-type layers, this is achieved by locating the origin of the stacking vectors at a rotocentre* and by making the rotation axes of the sheet cross the stacking vectors at their middle point; this corresponds to the location of the sheet centre over the middle of the square defined by the stacking vectors (Fig. 1).

Standard rectangular transparent sheets

The rectangular-shaped sheets have three rotation axes: two on their own plane and another perpendicular to it (Fig. 1).

In the case of $p4m$ layers there are mirror lines in two perpendicular directions, therefore, all these rotations are permissible. Starting with position A, position α is obtained by rotation about the diad axis I. The choice of the origin at the fourfold rotocentre and the location of the sheet centre makes the displacement vector associated with this rotation equal to the stacking vector $\mathbf{A}\alpha$. In a similar way position β is produced by rotating the sheet about the diad axis II, and position B by combining both rotations, or by using the diad axis normal to the plane of the sheet. Therefore, only one sheet is required to represent all possible positions for the regular stackings.

The four stacking positions are specified by letters inscribed in the sheet corners, the upper left-hand corner being taken as reference. Any letter identifies a stacking position only when brought to this reference corner. A standard sheet placed in a certain stacking position is specified by the letter referring to this position, followed by the other letters listed according to a clockwise sequence, and all enclosed within square brackets.

When marking on the pattern of the packed atoms the interstices corresponding to the various stacking modes, four different sheets will be generated. If we consider first the stacking f ($\frac{1}{2},\frac{1}{2}$ translation) and start with a sheet in position A, $[A\alpha B\beta]$, and mark the interstices defined by stacking over it a second sheet placed in position B, $[B\beta A\alpha]$, we obtain the four different relative positions: B over A, β over α, A over B and α over β. This grouping of the corner letters results from the coherency among the stacking positions, and covers all the possible combinations of the positions by this way of stacking. The complete standard sheet, with packed atoms and interstitial sites, is designated by $[A_B\alpha_\beta B_A\beta_\alpha]$, thus emphasizing by subindices the stacking positions to be placed immediately above, and which define the marked interstices. For the stacking s (0,0 translation) only one sheet is necessary $[A_A\alpha_\alpha B_B\beta_\beta]$, and for the stacking b, with two possible translations $0,\frac{1}{2}$ or $\frac{1}{2},0$, two sheets are necessary, $[A_\alpha\alpha_A B_\beta\beta_B]$ and $[A_\beta\alpha_B B_\alpha\beta_A]$ respectively. The simplest case of a $p4m$ layer, the square layer parallel to the (001) plane of cubic closest packing, has already been studied (Figueiredo & Lima-de-Faria, 1972, 1977).

In layer patterns with symmetry $p4g$, the rotation axes of the sheet coincide with glide lines. As a consequence, every axis produces a translation along itself. Only one sheet generates the four stacking positions, as for the previous case, but the sheet is now $[A\beta B\alpha]$ instead of $[A\alpha B\beta]$. By marking the interstices, four complete standard sheets are derived (Fig. 1). An example of a square-type layer with $p4g$ symmetry is the $\mathbf{N}^{21}$ layer (Lima-de-Faria & Figueiredo, 1976), which appears in several structures, mainly alloys, *e.g.* $Cu^{\overline{cb}}[Al_2]^{N_f^{21}}$, $Tl'Tl^{\overline{cb}}[Se_2]^{N_f^{21}}$, $Ni^pAl^{cb}[Al_2]^{N_s^{21}}$, where $\overline{cb}$ means anti-cubic void, t, tetrahedral void, p, prismatic void, and cb, cubic void. A rectangular standard sheet of a $\mathbf{N}^{21}$ layer corresponding to the stacking f is shown in Fig. 2. The interstices are of three kinds: distorted anti-cubic ($r_{\overline{cb}}=0{\cdot}693R$, where R means the radius of the packing atoms), square ($r_{sq}=0{\cdot}414R$), and two types of distorted tetrahedral interstices ($r_{t_1}=$

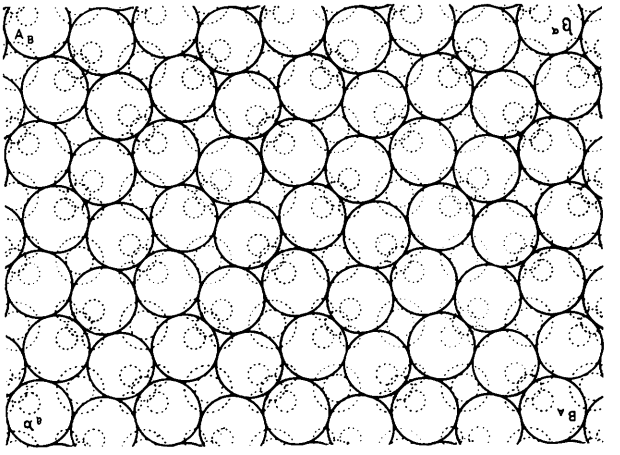

Fig. 2. Standard sheet, on a reduced scale (actual size of full circles $R=1$ cm) of a $\mathbf{N}^{21}$ layer showing the relative positions A_B, β_α, B_A and α_β, which correspond to the stacking f. Packed atoms are represented by full circles; large dotted circles correspond to distorted anti-cubic interstices, dotted circles concentric with these correspond to square voids, and the other dotted circles represent two categories of distorted tetrahedral interstices.

* Designation introduced by Le Corbeiller & Loeb (1967) which we prefer to 'rotation point' adopted in *International Tables for X-ray Crystallography* (1969).

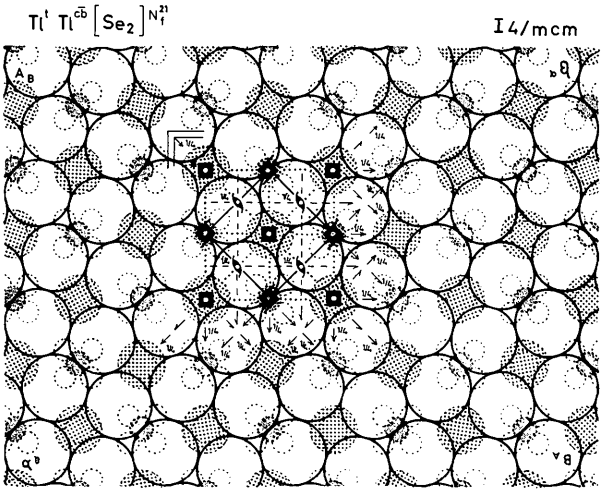

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Fig. 3. Sheet No. 1 of the condensed model of thallium selenide. Selenium atoms are represented by full circles forming N^{21} layers; thallium atoms correspond to filled circles, the smaller having tetrahedral coordination and the larger anti-cubic coordination. The unit cell (origin at level of the centres of packed atoms) and the elements of symmetry belonging to this sheet are also marked.

$0{\cdot}366R$ and $r_{t_2}=0{\cdot}311R$). There are half as many anti-cubic, square and larger tetrahedral voids as packing atoms, and twice as many of the smaller tetrahedral voids as packing atoms. The first sheet of the condensed model for the $Tl^{t}Tl^{\bar{cb}}[Se_2]^{N\frac{21}{1}}$ structure is shown on Fig. 3.

No symmetry lines exist on layers with symmetry *p*4, and rotations about the diad axes I or II produce enantiomorphous patterns, and, therefore, no possible positions. Only the diad axis perpendicular to the plane of the sheet can produce a new position because the pattern is then congruent. Each sheet can represent only two stacking positions, and therefore a total of eight standard sheets is necessary for the *p*4 patterns (Fig. 1).

Square transparent sheets

The symmetry operations of a square-shaped transparent sheet include two groups of diad axes on the plane of the sheet and a fourfold axis normal to it (Fig. 1). Thus, by fully using the two faces of the sheet each corner may represent two stacking positions, and therefore eight orientations of the sheets are possible.

Mirror and glide lines inclined at 45° are present in layer patterns with symmetries *p*4*m* and *p*4*g*, thus allowing the use of rotation axes III and IV of the square-shaped sheet. Moreover, in *p*4*m* patterns the rotation axis III coincides with a mirror line, and rotation axis IV with a glide line. In *p*4*g* patterns the reverse is true. Every one of the four stacking positions that were already obtainable with only one rectangular sheet appears twice in a square sheet because of this diagonal mirror line. The superposition of the pattern of interstices over the pattern of the packing atoms may destroy this mirror line and the corresponding rotation axis becomes operative. As a consequence only three sheets are required for symmetries *p*4*m* and *p*4*g*, in order to obtain all the modes and possibilities of stacking (Fig. 1).

In the case of layer patterns with symmetry *p*4, the existence of a fourfold rotation axis perpendicular to the square sheets allows the generation of the four stacking positions with the same sheet. As the rotation axes coplanar with the sheet are forbidden because they reverse the pattern, the permissible symmetry operations of the sheet are exhausted in this first process of generating the four stacking positions. If we now mark the pattern of the interstices for the normal stacking modes, four standard sheets are necessary to produce all the possible situations (Fig. 1).

The minimum set of standard sheets required to represent any sequence of square-type layers is therefore larger for the rectangular-shaped sheets than for the square-shaped ones. Nevertheless, the rectangular shape is more suitable for standardization purposes because the elaboration of a condensed-models file covering the various ideal structure types with many different symmetries would become very complicated with the use of different shapes for the standard sheets (square, hexagonal, rectangular, *etc.*), and consequently, of different supporting racks for their display. However, square-shaped sheets may be appropriate for building the condensed model of a particular structure if one does not intend to develop such a file.

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