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Concerning Systems for the Generating and Coding of Layered, Tetrahedrally Close-Packed Structures of Intermetallic Compounds

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Planar, tetrahedrally close-packed structures containing pentagon-triangle primary nets are analyzed on the basis of their secondary-net tessellations and geometry. Included are: (1) the structures generated and coded by Pearson and Shoemaker containing secondary-net tessellations of 4^4 , 3^6 , $3^4 4^2$, and $3^2 4^3 4$; (2) the structures derived by Kripyakevich in which secondary-net tessellations of $3^4 4$ and $3^5 4$ occur; and (3) some structures, generated here for the first time, with some secondary-net tessellations of 3^5 . We have extended the coding scheme of Pearson and Shoemaker to describe the second group of structures. It becomes complicated for structures with secondary nets that are not based on two sets of parallel lines. However, the simpler code proposed by Kripyakevich does not uniquely define these structures. Neither coding scheme adequately describes the third group of structures.

Introduction

'Tetrahedrally close-packed' (t.c.p.) structures are structures in which all atoms have interpenetrating triangulated coordination polyhedra with coordination numbers (C.N.) 12, 14, 15 or 16, and in which all interstices are tetrahedral. Many of the known examples of t.c.p. structures are 'planar'; that is, they are generated by the alternate stacking of main (primary) layers, in mirror planes, consisting of hexagon- and/or pentagon-triangle nets of atoms and subsidiary (secondary) layers which are less dense and consist of triangle, rectangle-triangle, or rectangle nets between the mirror planes. The pentagons and the hexagons of the primary nets are covered antisymmetrically by the pentagons and hexagons of the neighboring primary nets, and the atoms of the interleaving secondary nets center (in projection) all the pentagons and hexagons of the primary nets.

In Fig. 1, projections are shown of fragments of structures which have primary nets consisting in (a) of

hexagons and triangles and in (b) of pentagons and triangles. The secondary nets in these two cases differ in geometry. They consist in (a) of (approximate) squares and (approximately) equilateral triangles, and in (b) of rectangles (ratio of the two sides about $\sqrt{3}/2$) and of isosceles triangles with two angles of about 55° and one angle of about 70° (Shoemaker & Shoemaker, 1969). The polyhedra surrounding the atoms of the secondary nets in (a) share triangular faces perpendicular to all edges of the squares and triangles in the secondary net, and in (b) share triangular faces perpendicular to the *short* edges of the triangles and rectangles, but share edges in the planes perpendicular to the *long* edges of the net. To emphasize this asymmetry in the secondary nets of pentagon structures we will indicate the long edges of the nets by full double lines and the short edges by full lines. (These lines connect second-nearest neighbors and do not represent bonded contacts.)

In analyzing possible t.c.p. structures it is convenient to consider the possible configurations of the secondary

nets. As has been pointed out by Pearson & Shoemaker (1969), referred to as P & S in the following, the entire structure may be generated once the configuration of the secondary net, and the sequence of pentagons and hexagons in the primary nets, are known. In Fig. 2 the tessellations with the Schläfli symbols that may occur in the secondary nets of structures with hexagon-triangle primary nets are shown on the left, and the corresponding ones for pentagon-triangle primary nets are shown on the right, with examples of structures in which they occur. The tessellations $3^4 4$ and $3^5 4$ can only occur in pentagon structures and have recently been found in the structure of the X phase, occurring in the Mn-Co-Si system, by Yarmolyuk, Kripyakevich & Hladyshevskii (1970) and independently by Manor, Shoemaker & Shoemaker (1972). (The secondary nets in the X phase are not strictly planar, but this does not change the angles substantially.) The second types of $3^4 2$ and $3^2 4 3 4$ tessellations for pentagon structures are hypothetical, but could certainly occur since they do not imply serious distortion of the coordination polyhedra. The 3^5 tessellation is postulated here for the first time for t.c.p. structures, and will be further considered below.

Structures with pentagon-triangle primary layers and secondary nets based on parallel zigzag lines

The derivation of possible secondary nets for pentagon-triangle primary nets consists of fitting together

rectangles and isosceles triangles of the above described geometry. It is convenient to divide the nets into strips running in the Y direction (at an angle between 0 and 30° with the vertical), consisting of rectangles and pairs of two triangles. In these strips we will, whenever possible, place the rectangle with its long edge approximately in the Y direction. Fig. 3 shows how two triangles in such a strip may be combined to form what we will henceforth refer to as a 'parallelogram', a 'rhomb' (rh) or a 'quadrangle' (qu). P & S only considered nets which had vertical strips consisting of rectangles and pairs of triangles forming parallelograms. An example of such a structure is given in Fig. 4, which is the pentagon analog of the σ phase. The simplified code for this structure, derived by P & S, is: $P(+ - ; LR)$, in which P indicates that the primary net contains pentagons only (no hexagons) and the expression in parentheses indicates the configuration of the secondary net: $+ -$ indicates that the zigzag lines in the horizontal direction go alternately up and down; LR indicates that the zigzag lines in the vertical direction are alternately sloped to the left and to the right.* The space group is $Pbam$, $Z=26$. Recently Kripyakevich & Yarmolyuk (1971) have assigned this structure to the compound $W_6(Fe, Si)_7$. All the structures considered by P & S could be generated by sets of parallel

* We use the symbols $+$ and $-$, rather than the numbers in the simplified code of Table 1 of P & S to avoid confusion with the symbols used by Kripyakevich (see below).

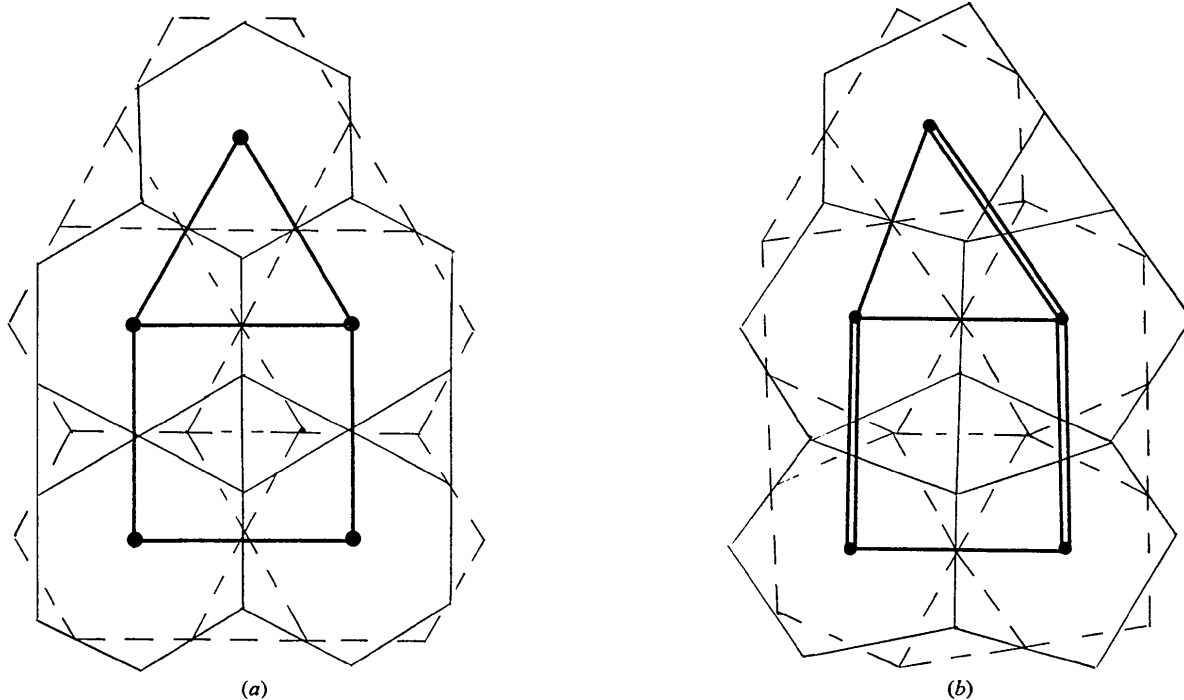


Fig. 1. (a) Fragment of a structure with hexagon-triangle primary layers and secondary layers consisting of squares and (approximately) equilateral triangles. (b) Fragment of a structure with pentagon-triangle primary layers and secondary layers consisting of rectangles and isosceles triangles. The longer edges of the secondary net are indicated by double lines.

lines and contained only the first four types of tessellations shown in Fig. 2.

Kripyakevich (1970), referred to as K below, derived and classified several series of structure types, mostly hypothetical, by combining fragments of the structures of Zr_4Al_3 and $MgZn_2$ (or $MgCu_2$), and called by that author 'homologous series'. In his derivations the

secondary-net triangles in the $MgZn_2$ structure were for simplicity assumed to be equilateral. Three of the series derived by him contain only the first four types of tessellations (including the second type of 3^34^2 tessellation) and are among the structures generated by P & S. They may be unambiguously described by the P & S coding scheme: the series based on Fig. 4(c)

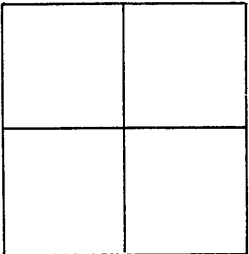
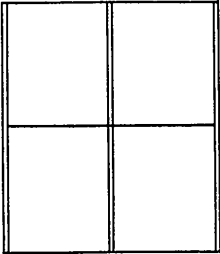
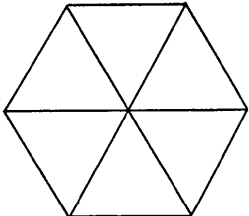
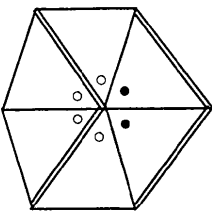
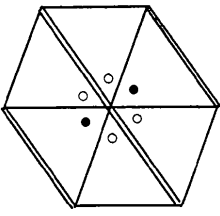
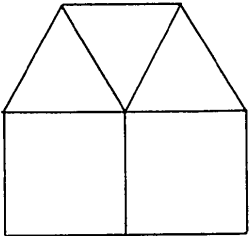
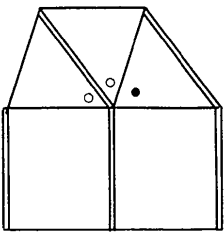
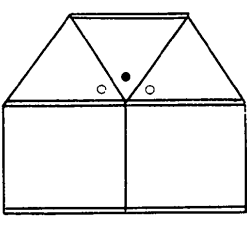
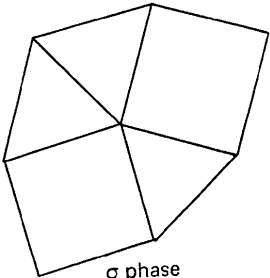
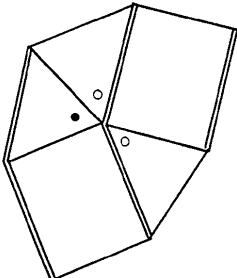
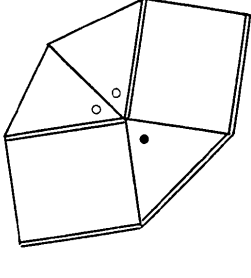
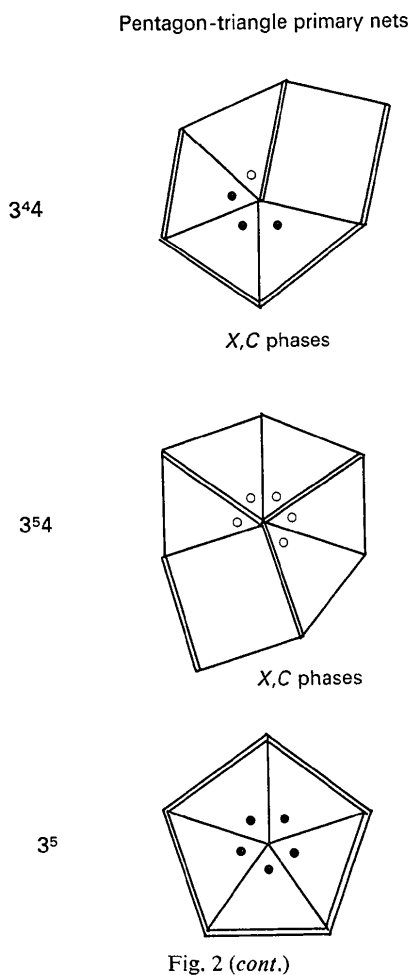
Secondary-net tessellations	Hexagon-triangle primary nets	Pentagon-triangle primary nets	
4^4	 β -W	 $Zr_4Al_3(110)$	
3^6	 $Zr_4Al_3(001)$, ν phase	 $MgZn_2$	 $MgCu_2$
3^34^2		 M, μ phases	
3^2434	 σ phase	 M phase	

Fig. 2. Tessellations that may occur in secondary nets of hexagon-triangle primary nets and pentagon-triangle primary nets with some examples of structures in which they occur. The solid dots indicate angles of approximately 70° , the circles angles of approximately 55° .



of K by using the notation *A* or *C* of Table 1 of P & S and the series based on Fig. 5(a) and (b) of K by notation *B* of Table 1 of P & S. Other types of homologous series were derived by K by constructing secondary nets out of 'ribbons', alternately consisting of what is called by him 'squares' and 'rhombs' (but which actually are rectangles and rhombs or parallelograms) and of 'rhombs' only (or actually rhombs and parallelograms).^{*} These new structures contain the tessellations 43⁴ and 43⁵ and are therefore not covered by the coding scheme of P & S. The short-hand notation given by K to these structures is: $(q, r)_s(q+r)_t$, in which *s* is the number of ribbons consisting of *q* 'squares' and *r* 'rhombs' and *t* is the number of ribbons containing $(q+r)$ 'rhombs'. Homologous series are produced by changing the values of *q* and *r*, or of *s* and *t*. Each symbol corresponds to two 'homeotypic' structures – one orthorhombic and one monoclinic – differing in the configuration of the ribbons of 'squares' and

* We will call the strips chosen by K 'ribbons', to distinguish them from the strips chosen by us, which may run in a different direction.

'rhombs'. These two structures are distinguished by adding the symbol \parallel and \perp , respectively. However, these symbols do not uniquely define the structures since no difference is made between parallelograms, rhombs and quadrangles. Reference to Fig. 7 of K is necessary to see the exact configuration of the ribbons. Also, for a particular structure it is not obvious in what direction the ribbons should be chosen.

Fig. 5 shows two examples of the new structures derived by K. We have drawn these structures so that the vertical strips contain rectangles and parallelograms in the same configuration as in Fig. 4, but now pairs of triangles that are combined to form rhombs also occur in these strips. A rhomb is introduced in a vertical strip such that a whole row of rhombs is gener-

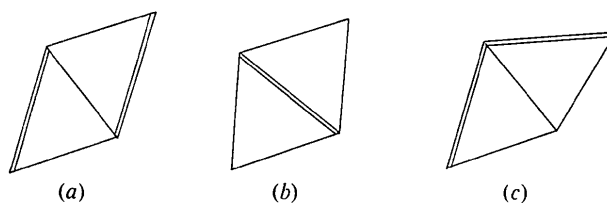


Fig. 3. Pairs of isosceles triangles in vertical strips may be combined to form (a) a parallelogram, (b) a rhomb (rh) or (c) a quadrangle (qu).

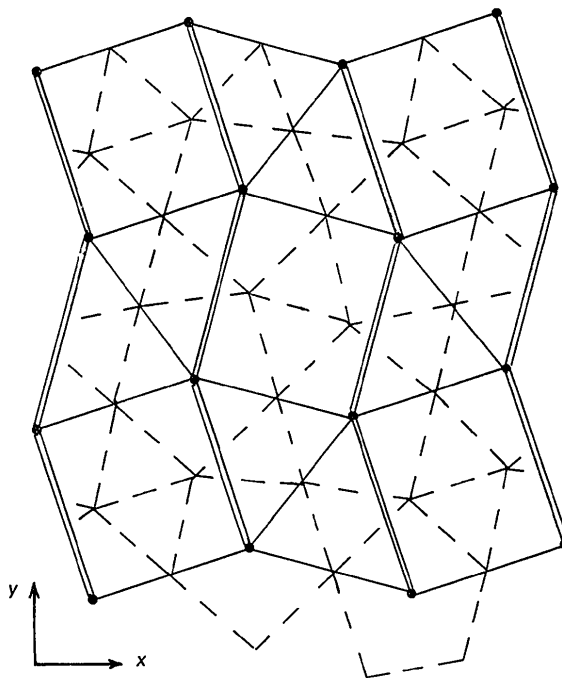


Fig. 4. Structure of $W_6(Fe, Si)_7$: $P(+ - ; LR)$. In this and following figures the secondary net is emphasized by full lines indicating short edges and full double lines indicating long edges. One primary net is outlined in broken lines; the pentagons of the next primary net are placed antisymmetrically over the pentagons of this net. K symbol: $(1, 1)_1$.

ated extending in the horizontal (**X**) direction. The vertical zigzag lines now contain a short edge wherever a rhomb has been inserted. Our original notation could be made applicable to these structures by indicating where a row of rhombs has been added, as for instance for the structure in Fig. 5(a): $P(+ - ; L, rh, R, rh)$, which indicates that it is the pentagon analog of the σ phase with two horizontal rows of rhombs inserted. K's symbol for this structure is (the ribbons run in horizontal direction): $(1, 1)_1 2_1 \parallel$. Our code for the structure in Fig. 5(b) is: $P\{+ - ; (L, rh)_2\}$, and K's notation (ribbons vertical): $(1, 1)_1 2_1 \perp$. The composition of both structures is R_2X_3 ,* the space groups are respectively

* The composition of a phase in terms of the numbers of the atoms with C.N. > 12 (R atoms) and atoms with C.N. = 12 (X atoms) is derived by K by counting the number n of rhombs (or parallelograms), which are parts of e.g. the $MgZn_2$ structure and thus contribute R_2X_4 , and the number m of rectangles, which are parts of the Zr_4Al_3 structure and thus contribute R_4X_3 , leading to the formula $R_{2n+4m}X_{4n+3m}$. Structures with the same ratio of R and X atoms are called 'homeotypic'.

$Pnmm$ and $A2/m$ (first monoclinic setting), and Z (the number of atoms per unit cell) is 50. Recently Kripyakevich & Yarmolyuk (1970) have found that Fig. 5(b) represents the structure of the C phase $V_2(Co_{0.57}Si_{0.43})_3$.

K's structure $(1, 1)_1 2_1 \parallel$ is given in Fig. 6(a); the composition is $R_{14}X_{23}$, $Z=74$, and the space group is $Pbam$. It is the pentagon analog of the σ phase with two consecutive rows of rhombs inserted: $P\{+ - ; L(rh)_2 R(rh)_2\}$. The structure of Fig. 6(b) is homeotypic; its space group is $P2/m$, $Z=37$. Notations: $(1, 2)_1 3_1 \perp$ and $P\{+ - ; L(rh)_2\}$.

A third structure of composition $R_{14}X_{23}$ is given in Fig. 7(a). Although it is uniquely defined by the symbol $P\{(+ - -)_2 ; (L, rh)_2\}$ its unit cell is actually smaller than indicated by this symbol, as shown by the choice of axes X', Y' rather than X, Y . Its space group in the latter axial system is $A2/m$, $Z=74$, and it is presumably K's structure $(1, 1)_1 2_1 \perp$. The shaded row in the X' direction represents a new type of basal row, which may be used to derive other structures.

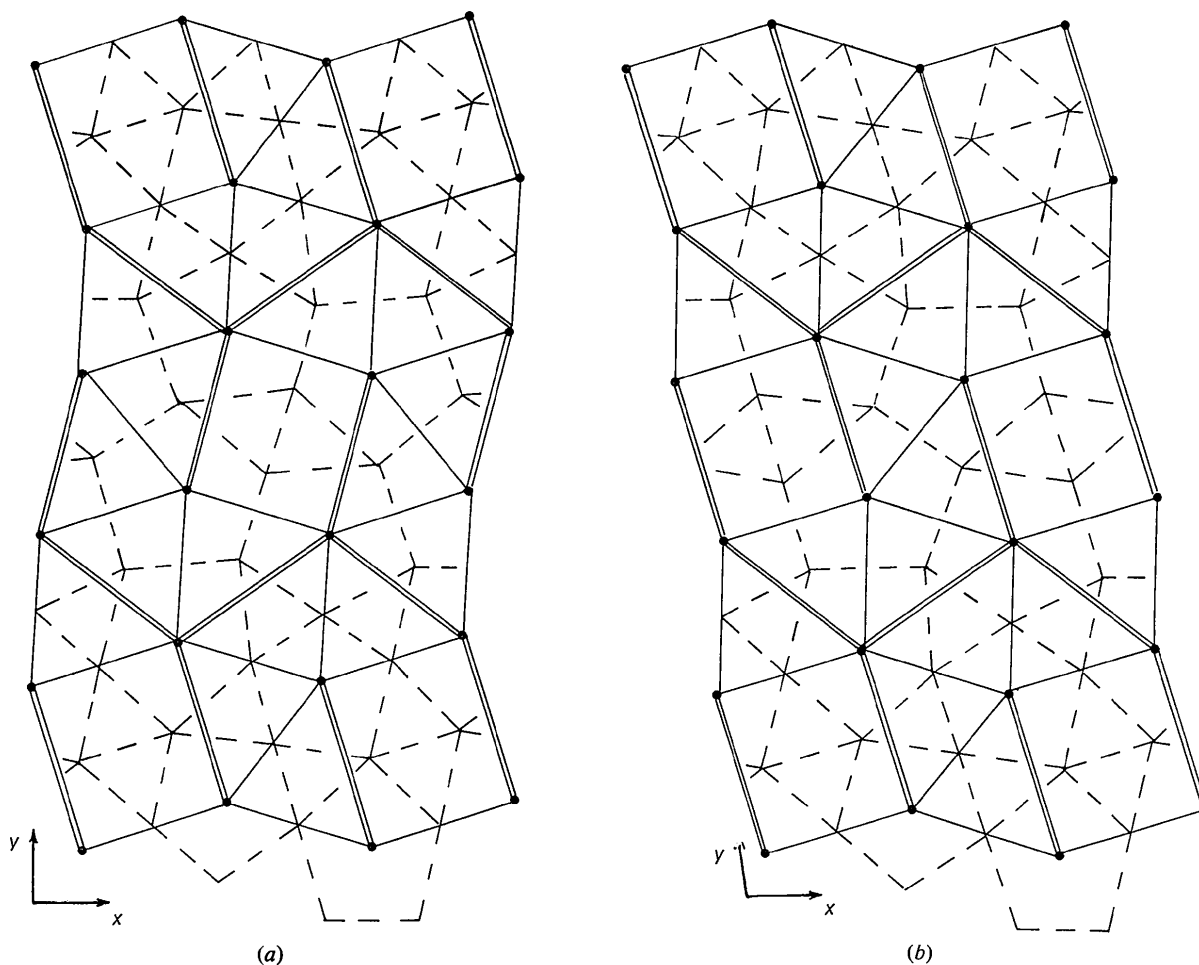


Fig. 5. (a) Hypothetical structure: $P(+ - ; L, rh, R, rh)$. Kripyakevich designation (ribbons horizontal): $(1, 1)_1 2_1 \parallel$. (b) The structure of the C phase: $P\{+ - ; (L, rh)_2\}$. Kripyakevich designation (ribbons vertical): $(1, 1)_1 2_1 \perp$.

Structures based on secondary nets of non-parallel zig-zag lines

Although these studies were inspired by the determination of the structure of the X phase, $R_{14}X_{23}$, none of the three homeotypic structures of that composition which we have described so far corresponds to the X -phase structure. In order to derive that structure we have to include in our vertical strips pairs of triangles forming 'quadrangles' [Fig. 3(c)] and indicate precisely

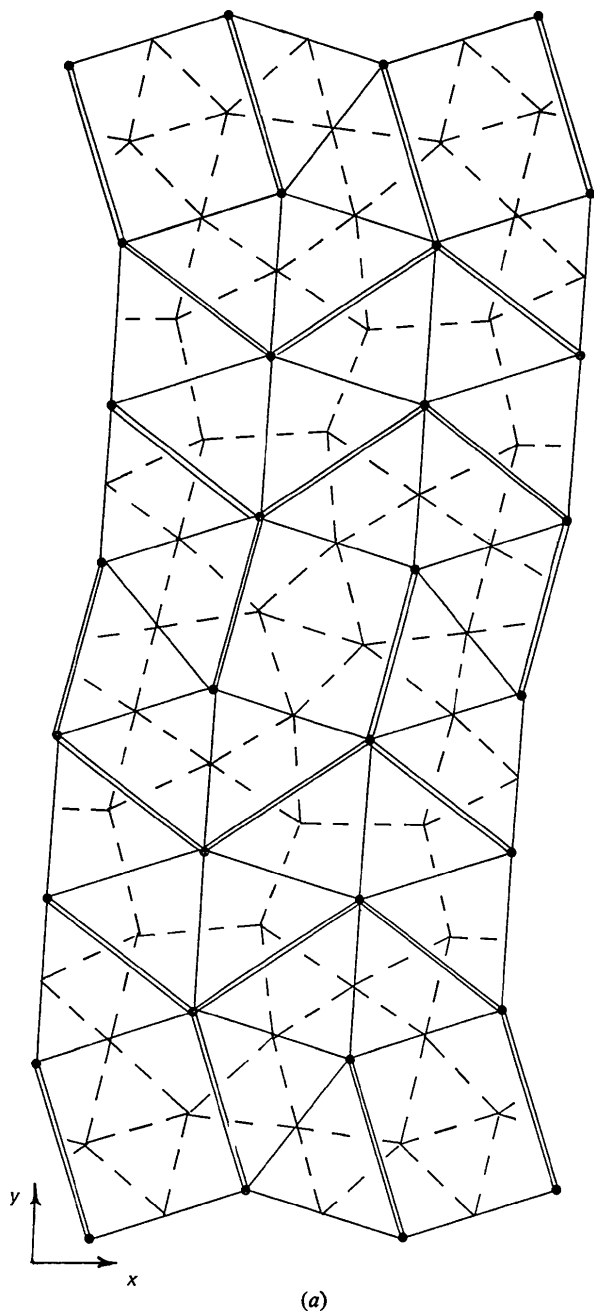


Fig. 6. (a) Hypothetical structure: $P\{+-; L(rh)_2R(rh)_2\}$. Kripyakevich designation (ribbons horizontal): $(1,1)_12_1\parallel$.

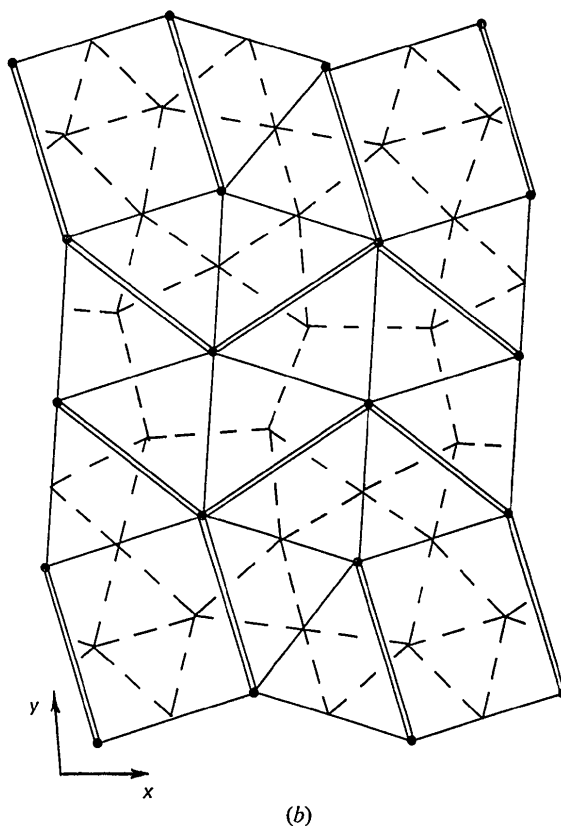


Fig. 6 (cont.). (b) Hypothetical structure: $P\{+-; L(rh)_2\}$. Kripyakevich notation (ribbons vertical): $(1,2)_13_1\perp$.

how the successive strips are built up. For instance the structure of Fig. 7(a) on the axial system X', Y could be defined by the symbol $P\{(L, rh)_2; (qu)_4; (qu)_4\}$, where now the compositions of successive strips in vertical direction are given. Fig. 7(b), which represents the structure of the X phase, could be defined as $P\{(R, (qu)_2, rh); (qu)_4; (qu, rh, L, qu)\}$.* (The space group for the X phase is $Pnmm$, $Z=74$.) These notations are now becoming very elaborate and are not very useful any more as shorthand codes. K's symbol for the X phase would be (ribbons horizontal) $(1,2)_13_1\parallel$, but this symbol would apply also for the structure given in Fig. 7(c). Our code for Fig. 7(c) would be: $P\{(+-)_2; L, rh, R, rh\}$. Composition R_2X_3 , $Z=150$, space group $B2/m (C_{2h}^3)$.

Structures with 3^5 tessellations of the secondary net

The study of the X phase has revealed that in planar t.c.p. structures with pentagon-triangle primary layers,

* It should be noted that the structure of a vertical strip is not uniquely defined by the part of the symbol referring to it, owing to different possible orientations of rh and/or qu; the unique definition depends also on necessary relationships between successive strips arranged as defined by the rest of the symbol.

tessellations of the type 43^4 and 43^5 can occur in the secondary layers without too much distortion of the coordination polyhedra. One might wonder if tessella-

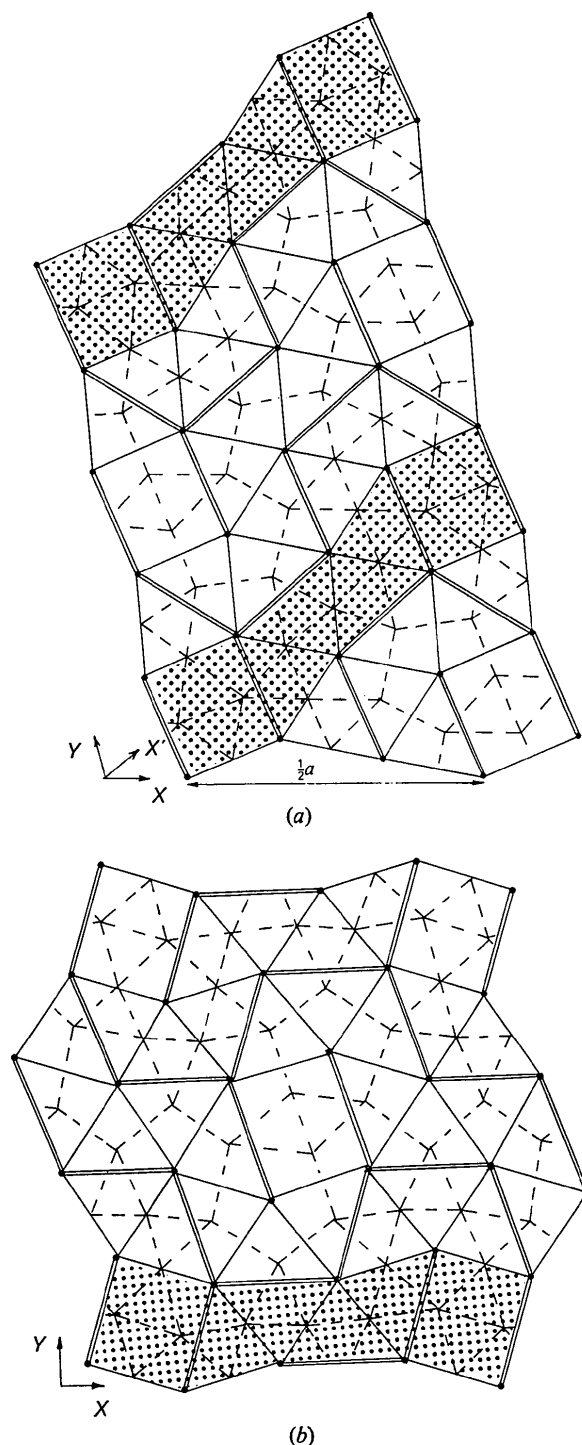


Fig. 7. (a) Hypothetical structure: $P\{(+ - -)_2; (L, rh)_2\}$. Kripyakevich designation (ribbons vertical): $(1,1)_2 \perp$. A smaller unit cell is obtained by using the shaded row as basal row. (b) The structure of the X phase. Kripyakevich notation (ribbons horizontal): $(1,2)_3 \parallel$. The shaded row is identical with the shaded row in Fig. 7(a).

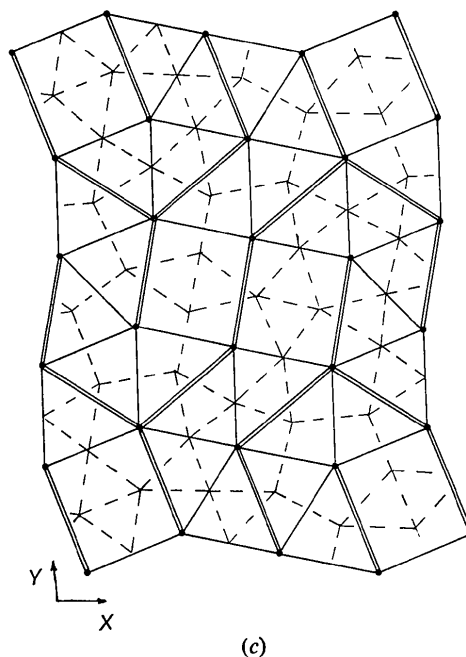


Fig. 7 (cont.). (c) Hypothetical structure $P\{(+ - -)_2; (L, rh, R, rh)\}$. Kripyakevich notation as in Fig. 7(b).

tions of the type 3^5 (Fig. 2) could also occur, formed by five isosceles triangles grouped together around a fivefold axis and thus forming angles of 72° (which is only about 2° larger than the angle occurring in the $MgZn_2$ -type structures). Starting with the shaded row in Fig. 7(a) a monoclinic structure may be constructed which contains some 3^5 tessellations of the secondary net, as shown in Fig. 8(a). Composition R_2X_3 , $Z=150$, space group $A2/m (C_{2h}^3)$.

A 3^5 tessellation is formed by five interpenetrating icosahedra alternating in the Z direction with five interpenetrating triangulated C.N. 16 polyhedra ('Friauf polyhedra'), each group of five polyhedra sharing an edge perpendicular to the net at the center of the pentagons. Additional vertical rows of interpenetrating icosahedra are formed, centered by the atoms of the secondary net. A finite group composed of five 'Friauf polyhedra' arranged this way with their complete first coordination shells (which include the five-membered rings of the C.N. 12 atoms above and below) is represented in Fig. 8(b). This complex, which contains 47 atoms, does occur as a building block in some of the complicated (mostly cubic) structures studied by Samson (1968), for instance in the structures of β - Mg_2Al_3 and $NaCd_2$. The complex is called by Samson the 'VF polyhedron' and is depicted by him as shown in Fig. 8(c), which follows from Fig. 8(b) by joining up the atoms in a different way. It is not known whether an arrangement as shown in Fig. 8(a), where five-rings of interpenetrating C.N. 16 polyhedra alternate with five-rings of interpenetrating icosahedra, forming an infinite stack, can indeed occur.

The structure in Fig. 8(a) might be defined as: $P\{(R, rh_3); (qu, rect, qu, rh); (qu, rh, qu, rect)\}$. The symbol 'rect' is used for a rectangle with its long edge approximately horizontal, and the symbols L and R are reserved for the rectangles with the long edges approximately vertical.

Fig. 9 shows three more hypothetical structures containing five-membered rings in the secondary layers. These structures also contain the second type of 3^2434 tessellation shown in Fig. 2. Fig. 9(a) contains X -phase type rows enclosing five-membered rings on mirror planes. The space group is $Cm2m (C_{2v}^{14})$, $Z = 112$, the composition is $R_{11}X_{17}$. The secondary net of Fig. 9(b), considered as consisting of pentagons, rectangles and triangles, is an example of a planar 4-connected net having pentagons, rectangles, and triangles in the ratio 1:1:1 (Wells, 1968). The examples of such 4-connected nets given by Wells cannot be used for the construction of our secondary nets because of our

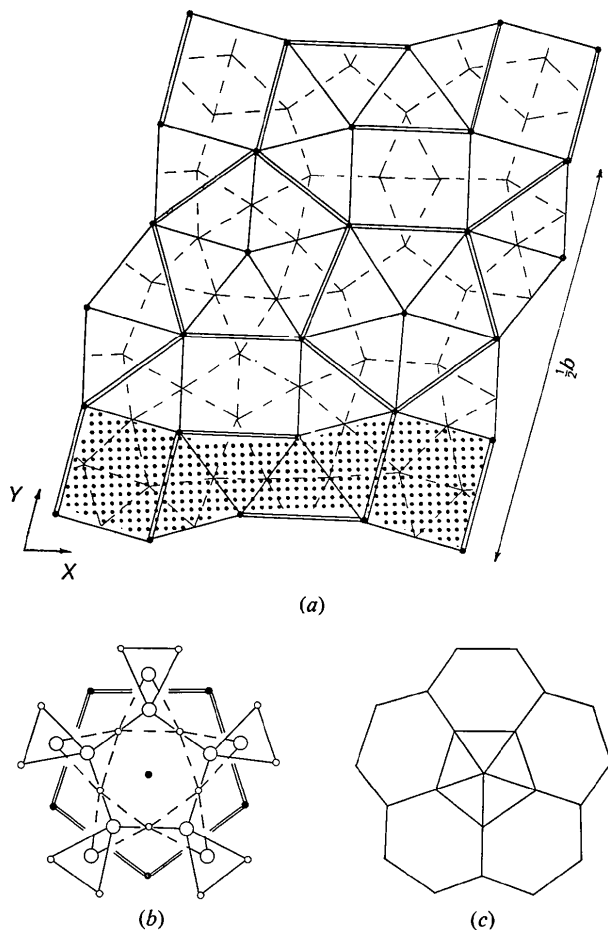


Fig. 8. (a) Hypothetical structure containing 3^5 tessellations of the secondary net. (b) Projection of Samson's VF polyhedron. Full lines connect atoms at $Z=0$, broken lines atoms at $z = \pm \frac{1}{2}$. Full circles represent atoms at $z = \pm \frac{1}{2}$; large circles C.N. 16 atoms, small circles C.N. 12 atoms. (c) Atoms in Fig. 8(b) connected to give Samson's representation of the VF polyhedron.

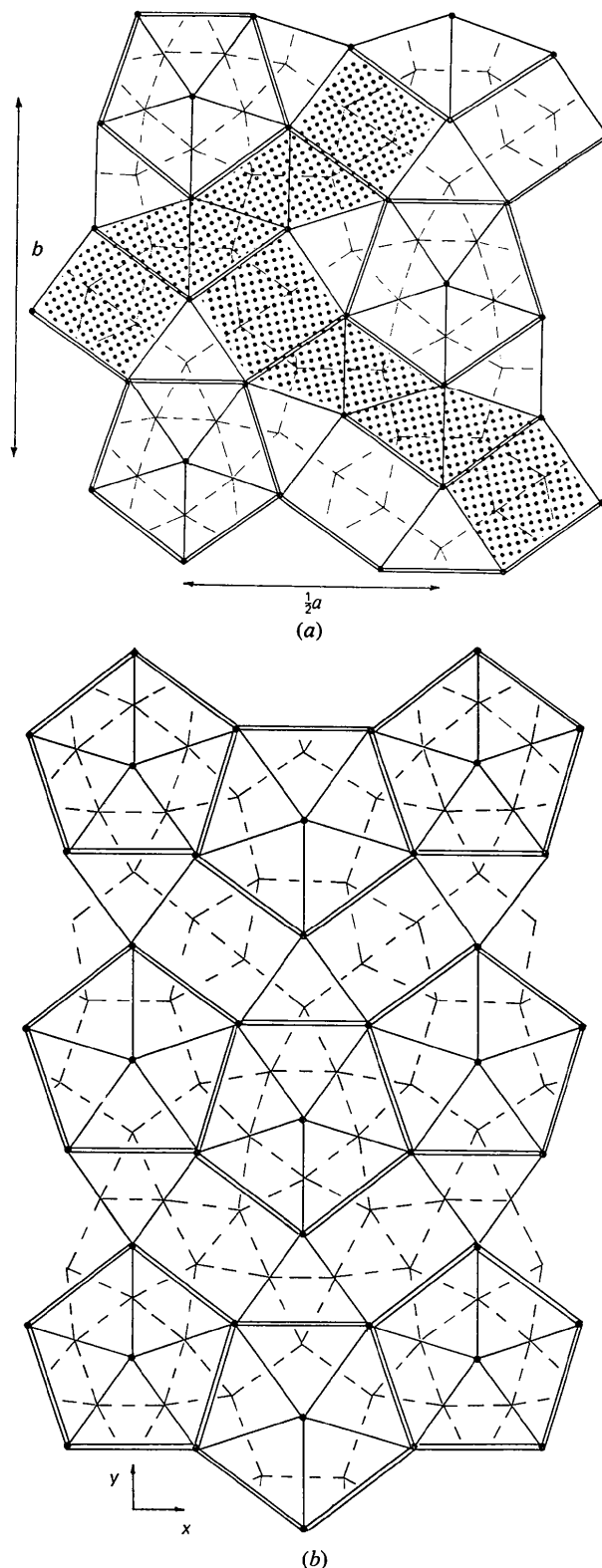


Fig. 9. (a) Hypothetical structure $R_{11}X_{17}$ with secondary-net pentagons (3^5 tessellations) on mirror planes $\perp X$. (b) Hypothetical structure R_2X_3 with secondary-net pentagons (3^5 tessellations) on mirror planes $\perp X$ and ratio of pentagons:rectangles:triangles = 1:1:1.

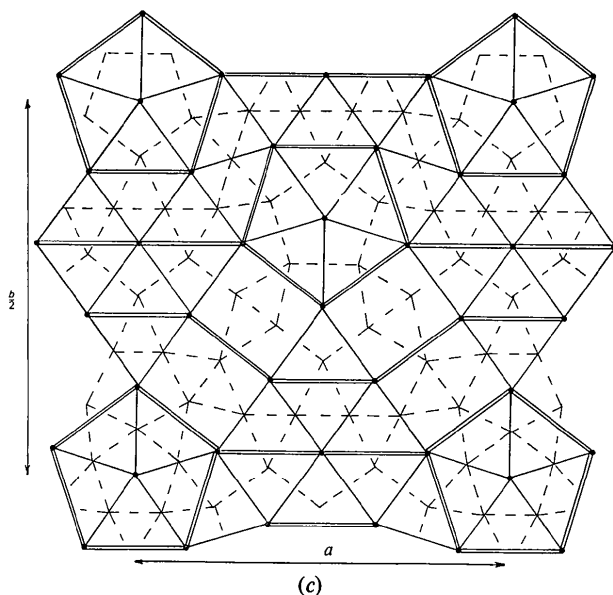


Fig. 9 (cont.). (c) Hypothetical structure $R_{11}X_{17}$.

restrictions that all edges of the pentagons should be long, that the rectangles should have two long edges, and that the triangles have only one long edge. The space group for the structure in Fig. 9(b) is $Amam (D_{2h}^{17})$, $Z=100$; the composition is R_2X_3 . In Fig. 9(c) the arrangement of the pentagons along the X axis is like the arrangement of the VF polyhedra in

β - Mg_2Al_3 along the [110] axis (Samson, 1968). The composition is $R_{11}X_{17}$, $Z=224$, space group $Amam$. Since there is no obvious way to divide these structures into strips, the derivation of code names becomes arbitrary and cumbersome. It is clear that many more structures of this type with larger cells could be derived. Both the P & S and the K coding scheme are clearly inadequate to describe these structures.

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The Crystal Structure of Tin(II) Iodide

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A complete structural analysis of tin(II) iodide (SnI_2) has been carried out on the basis of three-dimensional X-ray diffraction data and refined to an R value of 0.049. The crystals are monoclinic, space group $C2/m$, with $a=14.17$, $b=4.535$, $c=10.87$ Å, and $\beta=92.0^\circ$. The compound is shown to possess a unique AX_2 layer structure in which the metal atoms occur in two distinct sites. Two-thirds of the tin atoms occupy sites similar to those in $SnCl_2$ ($PbCl_2$ type). The remaining tin atoms are in $PdCl_2$ -type chains which interlock with the $PbCl_2$ -type part of the structure to give almost perfect octahedral coordination. Significant Sn-I distances are all in the range 3.00–3.25 Å. Mössbauer spectroscopy fails to reveal the true complexity of the structure.

Introduction

Detailed studies on the preparation of tin(II) iodides (to be published elsewhere) afforded crystals of SnI_2 suitable for single-crystal X-ray diffraction. Structural

analysis was carried out as part of a wider programme to extend the data on the crystal chemistry of tin(II). Aylett (1969) suggested that SnI_2 and PbI_2 have the same structure (CdI_2 type), while Belotskii, Antipov, Nadochii & Dodik (1969) found that SnI_2 and PbI_2 form a continuous series of solid solutions of PbI_2 (CdI_2) structure, pure SnI_2 having a 'different structure'.

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