Acta Crystallographica Section A
Foundations of Crystallography
ISSN 0108-7673

Zhdanov's rules work both ways

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Received 23 January 2006
Accepted 8 March 2006

The relationship between the space-group symmetry of a close packing of equal balls of repeat period P and the symmetry properties of its representing Zhdanov symbol is analyzed. Proofs are straightforward when some symmetry is assumed for the stacking, and it is investigated how this symmetry is reflected in the structure of the Zhdanov symbol. Most of these proofs are documented in the literature, with variable degrees of rigor. However, the proof is somewhat more involved when working backwards, *i.e.* when some symmetry properties for the Zhdanov symbol are assumed and the corresponding effect on the symmetry of the polytype structure it represents is investigated, which may explain why these proofs are avoided or shrugged off as 'easily seen', 'obvious' and the like.

1. Introduction

It is well known that any close-packed stacking of close-packed layers of equal balls (referred to in what follows as 'stacking' or 'polytype') can be represented by a Zhdanov symbol (Zhdanov, 1945, 1965), which consists of an even number of positive[1] integers, called 'components' in what follows, $n_1 n_2 n_3 \ldots n_{2k}$, such that $\sum n_i = P$, the repeat period of the stacking. The symbol represents n_1 layers stacked $\ldots A \rightarrow B \rightarrow C \rightarrow A \ldots$, followed by n_2 layers stacked $\ldots A \rightarrow C \rightarrow B \rightarrow A \ldots$ and so on, when we move along, say, the positive direction of the stacking axis. If we define $n_1 + n_3 + n_5 + \ldots = p$ and $n_2 + n_4 + n_6 + \ldots = q$, then for $p - q \equiv 0 \,(\mathrm{mod}\, 3)$ the lattice of the stacking will be hexagonal, otherwise it will be rhombohedral. The Zhdanov symbol uniquely represents the structure but the reciprocal statement is not true: the same structure can be represented by different Zhdanov symbols, *i.e.* the mapping between structures and Zhdanov symbols is a one-to-many mapping.

The relationship between the space-group symmetry of the stacking and the symmetry properties of the Zhdanov symbol was first established by Zhdanov (1945) in the form of a set of rules. Zhdanov's rules, as stated by Patterson & Kasper (1959), Verma & Krishna (1966) and Zhdanov himself (1945, 1965) appear to be necessary conditions: when a symmetry element is present in the structure of the sphere stacking, then 'it shows up in the Zhdanov symbol' (Patterson & Kasper, 1959) in a way prescribed by Zhdanov's rules. Apparently, it has been largely taken for granted that they are also sufficient conditions, *i.e.* the presence of a certain symmetry in the Zhdanov symbol necessarily implies certain other symmetry elements in the structure of the stacking thus represented.[2] The symmetry properties of the Zhdanov symbol are best understood when one remembers that the symbol represents a unit of repetition, and hence it is amenable to be represented graphically by imposing cyclic boundary conditions, as sometimes employed in other problems in geometrical crystallography (Patterson, 1944; Iglesias, 1981*a*,*b*). We use a cyclical representation of the Zhdanov symbol (referred to in what follows as CRZS) consisting of p black dots and q white dots equally spaced on a circle, *i.e.* placed at the points resulting from dividing a circle into $p + q$ equal parts (see examples in Fig. 1). We have established a mapping (see Table 1) between the space group of the sphere stacking represented by a Zhdanov symbol and the two-color point group of the CRZS, and assumed implicitly (Iglesias, 2006*a*) that the presence of certain symmetry elements in the CRZS (that is, in the Zhdanov symbol) necessarily implies certain other symmetry operations in the stacking thus represented. Since the Zhdanov symbols and the polytypes represented thereby are not in a one-to-one and onto relation, and since no explicit proof of the reciprocal

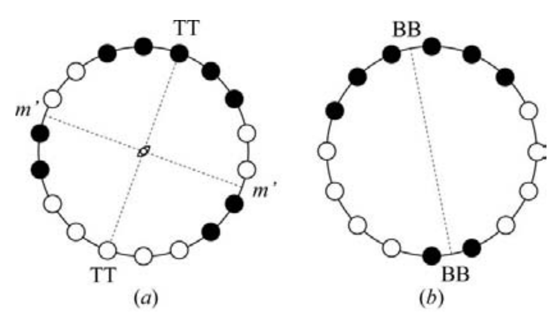

Figure 1
(*a*) CRZS of Zhdanov symbol 522522, showing anti-twofold rotor, *TT*-type mirror line and anti-mirror line. The point group is $2'mm'$ and the space group of the stacking is $P6_3/mmc$, with inversion centers at octahedral holes. (*b*) CRZS of Zhdanov symbol 6424, showing a *BB*-type mirror line. The point group of the CRZS is m and the space group of the stacking is $P\bar{3}m1$, with *S*-type inversion centers.

[1] The only exception is the f.c.c. packing, whose Zhdanov symbol is 10.
[2] Indeed, not even Zhdanov himself bothered to publish any proof of any of his own rules, and apparently he considered it obvious that they worked both ways, *i.e.* they were necessary and sufficient conditions.

symmetry relation between symbol and structure could be found in the literature, we shall endeavor in what follows to briefly prove this connection, and hence put our previous results (Iglesias, 2006*a*,*b*) on a firm basis. For each one of the rules contained in the old editions of *International Tables for X-ray Crystallography* (Patterson & Kasper, 1959), we make a direct translation into equivalent relations between the symmetry of the polytype structure and the two-color planar symmetry point group of the CRZS.

Table 1
Relationship between the symmetry group of the cyclic representation of the Zhdanov symbol, CRZS, and the space group of the stacking.

Two-color point group of CRZS	Space group of the stacking
No symmetry	$P3m1$, $R3m$
Mirror line only: point group m†	$P\bar{3}m1$, $R\bar{3}m$
Anti-mirror line only: point group m'	$P\bar{6}m2$
Anti-twofold rotor only: point group $2'$	$P6_3mc$
All three above: point group $2'mm'$‡	$P6_3/mmc$

† When the mirror line is of the *TT* type/*BB* type/*BT* type, the inversion centers are at octahedral holes (*O*)/spheres (*S*)/both (*SO*). ‡ The mirror line will be of the *TT* type/*BB* type if the half-period of the stacking, *P*/2, is odd/even.

2. Proofs of Zhdanov rules

2.1. Rule $\bar{1}(S)$

We reword Zhdanov's rule in the following way: 'A structure has a center of inversion at the center of a sphere (and hence all spheres in its close-packed plane will contain centers of inversion as well) if and only if the CRZS has a *B*-type mirror line[3] [*i.e.* a *BB* line or a *BT* line (Iglesias, 2006*a*)]'.

Proof

(*a*) Assume the structure has a center of inversion at the center of the spheres of an *A* layer. The argument given by Verma & Krishna (1966, p. 157) and the definition of a CRZS having a *B*-type mirror line can be taken to constitute a proof of this statement. It is to be noted that, after proving this, these authors give examples whose truth would require the proof of the converse implication, which they do not furnish.

(*b*) Assume the CRZS has a *B*-type mirror line (see Fig. 1*b*). This mirror line incides on no dot in its *B* extremity[4] on the CRZS and, hence, the number of black dots on one side of the line must equal the number of black dots on the other side, and the same thing will happen with the white dots. We remember that black and white dots represent respectively any of the passages $\ldots A\to B\to C\to A\ldots$ and any of the passages $\ldots A\to C\to B\to A\ldots$ and are equivalent to the + and − signs employed in the Hägg symbol (see, for instance, Verma & Krishna, 1966, p. 85). We begin with the two dots (we assume they are plus signs) closest to a *B* extremity of the *B* mirror line (which can be either *BB* or *BT* type), and assume there is in between, for instance, an *A* layer; we risk no loss of generality by making these assumptions. Now we shall add dots of the same color and successively consider what happens for each value of the total number *m* of black (+) dots, placed symmetrically at each side, or *n* white (−) dots equally arranged:

$$\begin{array}{lll} m=n=1 & \ldots C^+A^+B\ldots & \ldots B^-A^-C\ldots \\ m=n=2 & \ldots B^+C^+A^+B^+C\ldots & \ldots C^-B^-A^-C^-B\ldots \\ m=n=3 & \ldots A^+B^+C^+A^+B^+C^+A\ldots & \ldots A^-C^-B^-A^-C^-B^-A\ldots \end{array} \qquad (1)$$

From this we tentatively extract the following pattern:

$$\begin{array}{ll} \text{When} & \text{The sequence} \\ \left.\begin{array}{r} m\equiv 1\,(\mathrm{mod}\,3) \\ -n\equiv 1\,(\mathrm{mod}\,3)\end{array}\right\} & \Rightarrow \text{begins with } C \text{ and ends with } B \\ \left.\begin{array}{r} m\equiv 2\,(\mathrm{mod}\,3) \\ -n\equiv 2\,(\mathrm{mod}\,3)\end{array}\right\} & \Rightarrow \text{begins with } B \text{ and ends with } C \\ \left.\begin{array}{r} m\equiv 0\,(\mathrm{mod}\,3) \\ -n\equiv 0\,(\mathrm{mod}\,3)\end{array}\right\} & \Rightarrow \text{begins with } A \text{ and ends with } A. \end{array} \qquad (2)$$

We prove by induction that (2) holds for any *m* plus signs or any *n* minus signs. We assume that the rule is satisfied by a given sequence of *k* plus signs, and then increase *k* by one unit. Then,

if $k\equiv 0\,(\mathrm{mod}\,3)$ then $\ldots A\ldots A\ldots$ goes to $\ldots C^+A\ldots A^+B\ldots$ when *k* goes to $k+1$;
if $k\equiv 1\,(\mathrm{mod}\,3)$ then $\ldots C\ldots B\ldots$ goes to $\ldots B^+C\ldots B^+C\ldots$ when *k* goes to $k+1$; and
if $k\equiv 2\,(\mathrm{mod}\,3)$ then $\ldots B\ldots C\ldots$ goes to $\ldots A^+B\ldots C^+A\ldots$ when *k* goes to $k+1$,

which means that the relations are also satisfied by $k+1$ plus signs. Since this is true for *m* = 1, 2, 3, then it will be true for any *m*. In a similar way, we can prove that this holds for any *n* minus signs.

In what follows, we say that two sign sequences whose CRZS both have a *B*-type mirror line, as discussed above, have the same character if their corresponding *ABC* sequences start with the same letter, and likewise end with the same letter (not necessarily the same as the previous one). We next observe that adding one − sign to a sequence of + signs produces a sequence of the same character as that obtained by taking out one + sign; for instance, the sequence having three plus signs followed by one minus sign, all mirrored around the central *A* layer, has the same character as that having just two plus signs (equally mirrored):

$$\ldots B^-A^+B^+C^+A^+B^+C^+A^-C\ldots \qquad \ldots B^+C^+A^+B^+C\ldots$$

and, by the same token, adding a new − sign to the last sequence will produce a sequence of the same character as that having just one plus sign; and hence a sequence of the same character would have been obtained starting out with the first sequence of three plus signs by adding two minus signs at each end.

[3] A *B*-type mirror line passes through the midpoint of the arc between dots at both ends (*BB* type) or only at one end (*BT* type).
[4] Not to be confused with a *B* layer.

It is easy to convince oneself that the order in which the plus and minus signs are added is irrelevant, as far as sequence character is concerned. Suppose that we are given a sequence of m_1 plus signs followed by n_1 minus signs followed by m_2 plus signs followed by n_2 minus signs and so on, such that $\sum m_i = m$, $\sum n_i = n$. After $m_1 + n_1$ signs, the sequence has the same character as a sequence of $m_1 - n_1$ plus signs. We now add m_2 plus signs, obtaining a sequence with the same character as one having $m_1 + m_2 - n_1$ plus signs, and then add n_2 minus signs, so that we get a sequence with the same character as one having $m_1 + m_2 - n_1 - n_2$ plus signs. It is evident that when the process ends the only relevant parameter is $\sum m_i - \sum n_j = m - n$. Hence,

$$\left.\begin{array}{ll}\text{When} & \text{The sequence}\\ (m-n)\equiv 1\,(\mathrm{mod}\,3)\Rightarrow & \text{begins with } C \text{ and ends with } B\\ (m-n)\equiv 2\,(\mathrm{mod}\,3)\Rightarrow & \text{begins with } B \text{ and ends with } C\\ (m-n)\equiv 0\,(\mathrm{mod}\,3)\Rightarrow & \text{begins with } A \text{ and ends with } A\end{array}\right\} \tag{3}$$

is the general rule, which means that we can only get sequences having these three different characters; and these characters, satisfied by any sequence, define precisely the presence of a center of inversion at the center of each sphere in the initial A layer.

It can be seen that making $B(C)$ the central layer would result in the rule

$$\left.\begin{array}{ll}\text{When} & \text{The sequence}\\ (m-n)\equiv 1\,(\mathrm{mod}\,3)\Rightarrow & \text{begins with } A(B) \text{ and ends with } C(A)\\ (m-n)\equiv 2\,(\mathrm{mod}\,3)\Rightarrow & \text{begins with } C(A) \text{ and ends with } A(B)\\ (m-n)\equiv 0\,(\mathrm{mod}\,3)\Rightarrow & \text{begins with } B(C) \text{ and ends with } B(C).\end{array}\right\} \tag{4}$$

This completes the proof.

It should be clear that the above proof depends only on the properties of the B extremity of the mirror line, and hence is valid for both BB- and BT-type mirror lines. It is valid even in the limit of the CRZS becoming a straight line, *i.e.* in the case where the sequence constructed around the central A layer is finite or, being infinite, never becomes periodic.[5] However, to clarify how such a sequence may be placed on a CRZS, and hence made periodic, we shall give a few examples.

We consider, for instance, the sequence $\ldots A^+B^-A^-C^+A\ldots$ and try to bend it to construct a valid CRZS. One possible way is depicted in Fig. 2(*a*). Placing the central A layer of the given sequence at the position marked with an asterisk, we bend the sequence over itself, making both extreme A layers become one and the same. The result is Zhdanov symbol 22 ($P = 4$) representing a hexagonal stacking belonging to space group $P6_3/mmc$, whose CRZS has a BB-type mirror line [in addition to that, it shows a $2'$ anti-twofold rotor and an anti-mirror line, not explicitly represented in Fig. 2(*a*)]. Its layer sequence is

$$\begin{array}{c}\ldots\big|ACAB\big|ACAB\big|ACAB\big|ACAB\big|\ldots\\ \uparrow\ \ \uparrow\ \ \uparrow\ \ \uparrow\ \ \uparrow\ \ \uparrow\ \ \uparrow\ \ \uparrow\end{array}$$

and it can be seen that all A layers contain S-type centers of inversion (marked with arrows). Additionally, the B and C layers contain mirror planes normal to the stacking direction (see §2.4 below) and the 6_3 screw can be recognized (after one reads through §2.5) to be incident on the balls of the A layers.

We can also bend the sequence and introduce an extra dot, say black, to get Zhdanov symbol 23, $P = 5$, which gives the CRZS depicted in Fig. 2(*b*), where it is plain that the mirror line is of the BT type. Since $2 - 3 \equiv 2 \neq 0\,(\mathrm{mod}\,3)$, this stacking is rhombohedral and belongs to space group $R\bar{3}m$. We must realize that the ABC sequence of a rhombohedral stacking will show periodicity along the normal to the layers only if the dot sequence is trebled, and hence the layer sequence of this stacking can be obtained by starting with an A layer at the position marked with an asterisk in Fig. 2(*b*) (emphasized below with a double arrow) and rotating clockwise three complete turns of the CRZS:

$$\begin{array}{c}\ldots BCAB\big|ACABCBABCACBCAB\big|ACABCBABCACBCAB\big|ACAB\ldots\\ \downarrow\ \ \Uparrow\ \ \downarrow\ \ \uparrow\ \ \downarrow\ \ \uparrow\ \ \downarrow\ \ \uparrow\ \ \downarrow\ \ \uparrow\ \ \downarrow\ \ \uparrow\ \ \downarrow\ \ \uparrow\ \ \downarrow\end{array}$$

where we have included $2\frac{2}{3}$ unit cells, marked by vertical bars. We have flagged the S centers (layers 1, 6 and 11 in each unit cell) with arrows pointing up, and the O centers, at interlayers 3–4, 8–9 and 13–14 in each cell (see §2.2) with arrows pointing down. Notice that the given sequence $ABACA$ appears centered at the initial A layer of every unit cell; the sequences $BCBAB$ and $CACBC$ are translationally equivalent through the rhombohedral unit-cell translations. Notice also that every run of five layers contains one layer with S centers and an interlayer space with O centers: this information is accurately displayed by the BT line in the CRZS depicted in Fig. 2(*b*).

If we take a sequence beginning with a C and ending with a B of the kind we are dealing with in this section [see expression (1) above] and wrap it around a circle, we can obtain a valid CRZS by inserting an extra $+$ sign between the extreme B and the C, so the mirror line will be of the BT type; for such

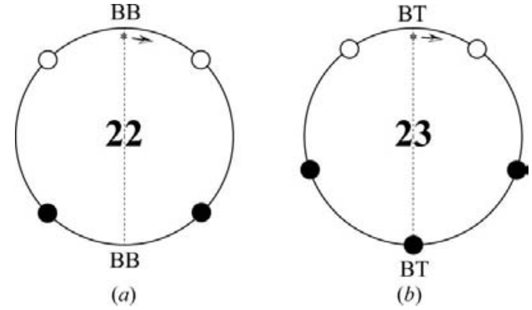

Figure 2
Two different CRZS both exhibiting the sequence $\ldots A^+B^-A^-C^+A\ldots$ We place the central A layer of the sequence at the position marked with an asterisk and choose as positive the sense of rotation described by the arrow. See §2.1(*b*) for details.

[5] In that case, the stacking would belong to one of the 80 diperiodic groups (Wood, 1964, p. 80) describing the symmetry properties of three-dimensional objects periodic only in two dimensions. In particular, the group would be $P\bar{3}2/m1$, No. DG72 in Wood's tabulation (Wood, 1964, p. 80).

a sequence [see equation (3)], we have $m - n \equiv 1 \pmod 3$ and hence the total balance of + and − signs is $2(m-n)+1 \equiv 0 \pmod 3$, and we get a Zhdanov symbol representing a hexagonal stacking. Similarly, a sequence starting with a B and ending with a C will give us a CRZS having a BT line if we introduce an extra − sign between the C and the B; and since for this $m - n \equiv 2 \pmod 3$, it can be seen that the sign balance is now $2(m-n)-1 \equiv 0 \pmod 3$ and, hence, that we get a hexagonal stacking as well.

Rhombohedral stackings with BB lines in the CRZS can be also obtained. Let, for instance, $\ldots C^-B^+C^+A^+B^+C^-B\ldots$, for which $m - n \equiv 1 \pmod 3$ [see equation (3)]. We construct a CRZS having four black dots and two white dots (Zhdanov symbol 42), and wrap the above sequence, placing the central A layer at the center point of the run of four black dots; after three turns around the circle, we get:

$$\begin{array}{l}\ldots CBC|ABCBABCABACABCACBC|ABC\ldots\\ \quad\;\uparrow\quad\uparrow\quad\uparrow\quad\uparrow\quad\uparrow\quad\uparrow\quad\uparrow\quad\uparrow\end{array}$$

where, again, the unit cell is marked by vertical bars and the S centers are marked with arrows pointing up. The reader can verify that only S centers are present here, consistent with the CRZS having a BB line.

2.2. Rule $\bar{1}(O)$

We rewrite this rule as: 'The polytype structure (*i.e.* the stacking) has a center of inversion at the center of an octahedral hole (and hence all octahedral holes in its close-packed plane will also contain centers of inversion) if and only if the CRZS has a T-type mirror line (*i.e.* a TT-line or a BT line)' (Iglesias, 2006*a*).[6]

Proof

(*a*) Assume the structure has a center of inversion at the center of the octahedral holes defined by two successive layers. Verma & Krishna (1966, p. 157) give an intuitive proof, which can be translated into the above rule when combined with the definition of a CRZS having a T-type mirror line (Iglesias, 2006*a*). Again, Verma & Krishna (1966, p. 157) use their examples as though the reciprocal property had been proven.[7]

(*b*) Assume the CRZS has a T-type mirror line (see example in Fig. 1*a*). Since such a line passes through a dot at its T extremity in the CRZS, this dot is the central dot of an odd run (an odd component of the Zhdanov symbol) of dots of the same color. We assume it represents the passage $A \to B$ (+ sign), or $B \to A$ (− sign):

$$\begin{array}{cc}\ldots A^+B\ldots & \ldots B^-A\ldots\\ \ldots C^+A^+B^+C\ldots & \ldots C^-B^-A^-C\ldots\\ \ldots B^+C^+A^+B^+C^+A\ldots & \ldots A^-C^-B^-A^-C^-B\ldots\end{array}$$

and if the number of +(−) signs in the central run is $m(n)$, necessarily odd, we can see that

$$\begin{array}{lll}\text{When} & & \text{The sequence}\\ \left.\begin{array}{r} m \equiv 1 \pmod 3\\ -n \equiv 1 \pmod 3\end{array}\right\} & \Rightarrow & \text{begins with } A \text{ and ends with } B\\ \left.\begin{array}{r} m \equiv 2 \pmod 3\\ -n \equiv 2 \pmod 3\end{array}\right\} & \Rightarrow & \text{begins with } B \text{ and ends with } A\\ \left.\begin{array}{r} m \equiv 0 \pmod 3\\ -n \equiv 0 \pmod 3\end{array}\right\} & \Rightarrow & \text{begins with } C \text{ and ends with } C.\end{array} \qquad (5)$$

The proof now follows the same lines as in the previous one, finally obtaining that the manufacture of a sequence in compliance with the T-type line of the CRZS produces ABC sequences necessarily belonging to one of the following characters:

$$\left.\begin{array}{lll}\text{When} & & \text{The sequence}\\ (m-n) \equiv 1 \pmod 3 & \Rightarrow & \text{begins with } A \text{ and ends with } B\\ (m-n) \equiv 2 \pmod 3 & \Rightarrow & \text{begins with } B \text{ and ends with } A\\ (m-n) \equiv 0 \pmod 3 & \Rightarrow & \text{begins with } C \text{ and ends with } C\end{array}\right\} \qquad (6)$$

where, out of m and n, one should be odd and the other should be even.

These relations specifically define the operation of a center of symmetry placed in the octahedral hole between an A and a B layer, which is frequently denoted as a γ site because it is located on the line perpendicular to the layers passing trough the spheres of a C layer. (*q.e.d.*)

2.3. Rule $\bar{1}(SO)$

We translate this rule into our jargon as: 'The structure has an inversion center at the center of an octahedral hole (and hence all octahedral holes in its close-packed plane will also contain inversion centers), together with a center of inversion at the center of a sphere (and hence all the spheres in its close-packed layer will also have this kind of inversion center) if and only if the CRZS has a BT-mirror line'.

Proof

Both direct and converse proofs are, obviously, combinations of the proofs given above for $\bar{1}(S)$ and $\bar{1}(O)$ and we shall omit the details, which can be easily reconstructed.

2.4. Rule for *m* parallel to the layers

We paraphrase this rule as: 'The polytype structure has a mirror plane parallel to the layers (which necessarily contains the centers of all spheres in a layer) if and only if the CRZS has an anti-mirror line (*i.e.* a two-color mirror line)'.

Proof

(*a*) Assume the structure has a mirror plane of this nature. We refer to Verma & Krishna (1966, p. 158) for an intuitive proof, which can be translated into the above rule when combined with the definition of a CRZS having an anti-mirror line (Iglesias, 2006*a*).

(*b*) We now assume the CRZS has an anti-mirror line (see example in Fig. 1*a*) and prove that the sphere stacking thus

[6] A T-type mirror line passes through the central dot of an odd run of dots of the same color at both ends (TT type) or only at one end (BT type).

[7] In fact, in this as in the other proofs these authors give, the proof of the direct statement is hopelessly entangled with that of the converse statement.

represented has necessarily a mirror plane contained in a layer. Since such an anti-mirror line passes necessarily between dots at both ends, the total number of black and white dots (+ and − signs) must be equal. We assume the anti-mirror line to represent sign symmetry around an A layer:

$$\begin{array}{cc} \ldots B^-A^+B\ldots & \ldots C^+A^-C\ldots \\ \ldots C^-B^-A^+B^+C\ldots & \ldots B^+C^+A^-C^-B\ldots \\ \ldots A^-C^-B^-A^+B^+C^+A\ldots & \ldots A^+B^+C^+A^-C^-B^-A\ldots \end{array}$$

Obviously the pattern now is

$$\begin{array}{ll} \text{When} & \text{The sequence} \\ \left.\begin{array}{r} m\equiv 1\,(\mathrm{mod}\,3) \\ -n\equiv 1\,(\mathrm{mod}\,3) \end{array}\right\} \Rightarrow & \text{begins with } B \text{ and ends with } B \\ \left.\begin{array}{r} m\equiv 2\,(\mathrm{mod}\,3) \\ -n\equiv 2\,(\mathrm{mod}\,3) \end{array}\right\} \Rightarrow & \text{begins with } C \text{ and ends with } C \\ \left.\begin{array}{r} m\equiv 0\,(\mathrm{mod}\,3) \\ -n\equiv 0\,(\mathrm{mod}\,3) \end{array}\right\} \Rightarrow & \text{begins with } A \text{ and ends with } A, \end{array} \tag{7}$$

where m (n) designates the number of + (−) signs at the right-hand side of the central A layer. We can prove, in analogy with the cases proved above, that the character of the sequences to be obtained when adding layers in accordance with the anti-mirror line is limited to

$$\left.\begin{array}{ll} \text{When} & \text{The sequence} \\ (m-n)\equiv 1\,(\mathrm{mod}\,3) \Rightarrow & \text{begins with } B \text{ and ends with } B \\ (m-n)\equiv 2\,(\mathrm{mod}\,3) \Rightarrow & \text{begins with } C \text{ and ends with } C \\ (m-n)\equiv 0\,(\mathrm{mod}\,3) \Rightarrow & \text{begins with } A \text{ and ends with } A \end{array}\right\} \tag{8}$$

which happens to be exactly what a mirror plane contained in an A layer (or, for that matter, any kind of layer) will produce.

2.5. Rule for 6_3 screw normal to the layers

Since the group of symmetry operations represented by a 6_3 screw contains the operations of a threefold axis of rotation as a subgroup, the location of a 6_3 screw normal to the layers of a close packing is restricted to the (possible) sphere positions for A, B and C kinds of layers (see, for instance, Figs. 18 and 20 in Verma & Krishna, 1966) because these are the places where the threefold axes are located (we remember that a sphere packing has minimum symmetry $P3m1$ or $R3m$). Every polytype, except h.c.p. (Zhdanov symbol 11) will have spheres at all three possible positions, hence the 6_3 screws will always contain some spheres. In h.c.p., the screw does not intercept any sphere, as it goes through the sphere positions of the unoccupied C-type layer (Verma & Krishna, 1966, p. 159). It is easy to see that a 6_3 screw passing through the spheres of a given layer type will generate another layer of the same type displaced by 1/2 along the screw (c) axis and layers of a different type will have symmetry-related mates, also displaced by 1/2, and having the type label exchanged. For instance, if the screw intercepts the spheres of an A layer, every layer in the unit cell will have a mate, generated by the screw axis, displaced by 1/2 along the c axis: those corresponding to A layers will also be A layers, those corresponding to B layers will be C layers, and those corresponding to C layers will be B layers.

We recast the corresponding Zhdanov rule as: 'The polytype structure has a 6_3 screw axis normal to the layers if and only if the CRZS has an anti-twofold axis of rotation, *i.e.* a two-color twofold rotor'. (See Fig. 1*a* for an example.)

Proof

(*a*) Assume the structure possesses such a screw axis. It is obvious, from the above discussion, that the second half of the unit cell along the c axis is entirely determined by the contents of the first half. We can suppose, with no loss of generality, that the screw is incident on the spheres of an A layer. We take the origin of the unit cell in this layer, so both the first and second halves start with an A layer. If the second layer of the first half is a B layer, the corresponding one in the second half will be a C layer, and reciprocally: it is clear that whatever sign, plus or minus, the first half starts with, the second one will start with the opposite sign:

$$\begin{array}{lll} |A^+B^-\ldots & |A^-C\ldots & | \\ |A^-C\ldots & |A^+B\ldots & |, \end{array} \tag{9}$$

where vertical bars are employed to mark the beginning of the two halves of the unit cell.

Suppose now that we start with A^+B and we add another layer; there are two possibilities:

$$\begin{array}{lll} |A^+B^-A\ldots & |A^-C^+A\ldots & | \\ |A^+B^+C\ldots & |A^-C^-B\ldots & |. \end{array} \tag{10}$$

It should be obvious by now that the sequence of signs we get in the second half of the unit cell is the negative of the sequence in the first half. This requires clearly that the total number of + and − runs in each half must be odd, since there must be a change of sign at the boundary between the two halves. Hence the corresponding Zhdanov rule: If the structure has a 6_3 screw, the Zhdanov symbol will consist of two equal halves, each containing an odd number of components. This immediately translates into a CRZS showing a two-color twofold rotor. (*q.e.d.*)

The proof offered by Verma & Krishna (1966, p. 159) is unclear and hardly convincing. Surprisingly, they add the sentence: 'The converse would also be true', with no further explanation.

(*b*) We now assume that the CRZS possesses an anti-twofold rotor and prove that this necessarily represents a stacking having a 6_3 screw. We consider, with no loss of generality, sequences starting with an A layer, satisfying an anti-twofold axis in its CRZS, *i.e.* the sequence of signs in the second half of the unit cell is the negative of that in the first half; we represent the jth layer in each half of the unit cell as X_j, Y_j such that $X_j, Y_j \in \{A, B, C\}$. Then, the unit cell can be represented as

$$\left|A^{s_1}X_2^{s_2}\ldots X_k^{s_k}\ldots X_n^{s_n}\right|Y_1^{t_1}Y_2^{t_2}\ldots Y_k^{t_k}\ldots Y_n^{t_n}\big|, \tag{11}$$

where

$$s_j, t_j \in \{+, -\} \quad \text{and} \quad s_j = -t_j, \quad 1 \le j \le n, \ n = P/2.$$

We call $S_k = \sum_{j=1}^{k-1}(s_j)1$, *i.e.* S_k is the difference between the number of plus signs and minus signs up to (but not including) layer number k and likewise define $T_k = \sum_{j=1}^{k-1}(t_j)1$, from which, obviously,

$$S_k = -T_k, \quad \forall k. \tag{12}$$

In §2.1 we have proved (3), which can be translated immediately into

$$\left.\begin{array}{ll} S_k \equiv 0\,(\mathrm{mod}\,3) & \Rightarrow \\ S_k \equiv 1\,(\mathrm{mod}\,3) & \Rightarrow \\ S_k \equiv 2\,(\mathrm{mod}\,3) & \Rightarrow \end{array}\right\} \text{layer } X_k \text{ is a} \left\{\begin{array}{l} A \text{ layer} \\ B \text{ layer} \\ C \text{ layer} \end{array}\right\} \tag{13}$$

and, in particular,

$$\left.\begin{array}{ll} S_{n+1} \equiv 0\,(\mathrm{mod}\,3) & \Rightarrow \\ S_{n+1} \equiv 1\,(\mathrm{mod}\,3) & \Rightarrow \\ S_{n+1} \equiv 2\,(\mathrm{mod}\,3) & \Rightarrow \end{array}\right\} \text{layer } Y_1 \text{ is a} \left\{\begin{array}{l} A \text{ layer} \\ B \text{ layer} \\ C \text{ layer} \end{array}\right\}. \tag{14}$$

Suppose, for instance, that $S_{n+1} \equiv 0\,(\mathrm{mod}\,3)$, hence layer Y_1 is an A layer. Clearly, any layer Y_k for which $T_k \equiv 0\,(\mathrm{mod}\,3)$ will also be an A layer and, by virtue of (12), the corresponding X_k layer in the first half of the unit cell will also be an A layer. Any X_k layer for which $S_k \equiv 1\,(\mathrm{mod}\,3)$ will be a B layer, as required by (13), and the corresponding Y_k, displaced by 1/2 along the c axis, will be a C layer due to (12); reciprocally, any X_k layer for which $S_k \equiv 2\,(\mathrm{mod}\,3)$ will be a C layer, and the corresponding Y_k, displaced by 1/2 along the c axis, will be a B layer. But this is [see part (*a*) of this proof] the hallmark of a 6_3 screw axis through the nodes of an A layer. The argument can be repeated assuming $S_{n+1} \equiv 1(2)\,(\mathrm{mod}\,3)$, and we will find 6_3 screws through the nodes of a $B(C)$ layer. Obviously, the nature of the 6_3 screw is a matter of definition and depends on the choice of origin.

This completes the proof.

3. Concluding remarks

The rules enunciated by Zhdanov relating the symmetry of a close-packed stacking of equal spheres and the symmetry properties of its Zhdanov symbol turn out to be, indeed, necessary and sufficient conditions. The best way to describe the symmetry properties of the Zhdanov symbol is to interpret these properties in terms of the two-color point group of symmetry of the cyclical representation of the Zhdanov symbol. The set of symmetry elements mapped out by this bijection is (Iglesias, 2006*a*) that described in Table 1.

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