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Symmetry of semi-reduced lattices

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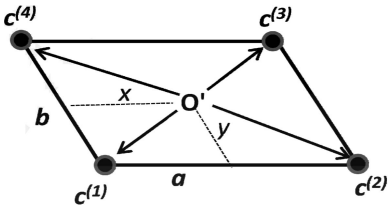
The main result of this work is extension of the famous characterization of Bravais lattices according to their metrical, algebraic and geometric properties onto a wide class of primitive lattices (including Buerger-reduced, nearly Buerger-reduced and a substantial part of Delaunay-reduced) related to low-restricted *semi-reduced descriptions* (*s.r.d.'s*). While the 'geometric' operations in Bravais lattices map the basis vectors into themselves, the 'arithmetic' operators in s.r.d. transform the basis vectors into cell vectors (basis vectors, face or space diagonals) and are represented by matrices from the set $\mathbb{V}$ of all 960 matrices with the determinant ±1 and elements $\{0, \pm1\}$ of the matrix powers. A lattice is in s.r.d. if the moduli of off-diagonal elements in both the metric tensors M and M^{-1} are smaller than corresponding diagonal elements sharing the same column or row. Such lattices are split into 379 s.r.d. types relative to the arithmetic holohedries. Metrical criteria for each type do not need to be explicitly given but may be modelled as linear derivatives $\mathbb{M}(p, q, r)$, where $\mathbb{M}$ denotes the set of 39 highest-symmetry metric tensors, and p, q, r describe changes of appropriate interplanar distances. A sole filtering of $\mathbb{V}$ according to an experimental s.r.d. metric and subsequent geometric interpretation of the filtered matrices lead to mathematically stable and rich information on the Bravais-lattice symmetry and deviations from the exact symmetry. The emphasis on the crystallographic features of lattices was obtained by shifting the focus (i) from analysis of a lattice metric to analysis of symmetry matrices [Himes & Mighell (1987). *Acta Cryst.* A**43**, 375–384], (ii) from the *isometric approach* and *invariant subspaces* to the *orthogonality concept* {some ideas in Le Page [*J. Appl. Cryst.* (1982), **15**, 255–259]} and *splitting indices* [Stróż (2011). *Acta Cryst.* A**67**, 421–429] and (iii) from fixed cell transformations to transformations derivable *via* geometric information (Himes & Mighell, 1987; Le Page, 1982). It is illustrated that corresponding arithmetic and geometric holohedries share space distribution of symmetry elements. Moreover, completeness of the s.r.d. types reveals their combinatorial structure and simplifies the crystallographic description of structural phase transitions, especially those observed with the use of powder diffraction. The research proves that there are excellent theoretical and practical reasons for looking at crystal lattice symmetry from an entirely new and surprising point of view – the combinatorial set $\mathbb{V}$ of matrices, their semi-reduced lattice context and their geometric properties.

1. Introduction

The work of Bravais (1850) – splitting the infinite set of three-dimensional lattices into 14 types and deriving for each type a primitive or centred translational cell, the symmetry of which is established by unique relationships between cell dimensions $(a, b, c, \alpha, \beta, \gamma)$ and is always the same as the symmetry of a given lattice – had a fundamental effect on the whole of geometric and practical crystallography, for example lattice classification, crystal structure standard description and analysis of structural crystal transitions. Two from three widely accepted levels of lattice classifications (de Wolff *et al.*, 1989) directly involve symmetry. The seven crystal systems are based on the conjugacy properties of the *geometric lattice groups*



within the orthogonal group $O(3)$. Classification into 14 Bravais types, on the other hand, is based on the conjugacy properties of the *arithmetic lattice groups* within the group $GL(3, \mathbb{Z})$ constituted by invertible 3×3 matrices with integer entries. The narrowest classes are defined by the reduced lattices (Minkowski, 1905; Niggli, 1928; Delaunay, 1933; Buerger, 1957) *via* metrical relationships. Each lattice in such a class shares the same arithmetic holohedry related to the Bravais lattices by the predefined transformations. The reduction formalism has rich algorithmic and mathematical support and leads to some generalizations [*e.g.* 127 genera obtained by Gruber (2006)]. However, in the presence of experimental errors it also suffers from *mathematical instabilities* (Andrews *et al.*, 1980). Several techniques were proposed to obtain higher perturbation stability (Andrews *et al.*, 1980; Grosse-Kunstleve *et al.*, 2004; Andrews & Bernstein, 1988, 2014; McGill *et al.*, 2014; Oishi-Tomiyasu, 2012). It should be noted that: (i) improvements in the *metric approach* lead to quite sophisticated algorithms, (ii) the concept of nearly Buerger-reduced lattices is useful for stability consideration, (iii) explicit criteria for 'lattice characters' or '*symmetrische sorten*' are valid for wider classes of lattices than accordingly reduced.

The dilemma of metric classification in the presence of experimental errors is unimportant if the arithmetic symmetry is determined, since primitive-to-Bravais transformations can be derived from a geometric interpretation of integer matrices. Le Page (1982) proposed searching lattice orthogonalities for arithmetic holohedry derivation. His *geometric approach*, so simple and stable, was incorporated in several computer programs for finding lattice symmetry (*e.g.* Cooper *et al.*, 2002). The method was originally used for Niggli-reduced cells, but is valid for an undefined wider class of lattices. In the *matrix approach* based on matrices which relate any primitive cell of the lattice to itself (Santoro *et al.*, 1980; Mighell *et al.*, 1981; Himes & Mighell, 1987; Karen & Mighell, 1989) the reduction step is completely omitted, but in the case of highly skewed cells a huge number of potential lattice relations should be tested, which creates the possibility of missed symmetries.

It has also been noted by several authors that for detailed analysis and 'keeping track of the symmetry changes in the lattices when their bases are deformed' (Pitteri & Zanzotto, 1998 and references contained therein) a non-standard description of metric symmetry by *arithmetic holohedries* is preferable over the *geometric holohedries* related to Bravais lattices. However, a matrix in the arithmetic holohedries is not an arbitrary invertible matrix and generally it is also not orthogonal (Kopský, 2001). Moreover, such a matrix is understood as an isometric operation only with the known lattice context (Hahn, 2006; Wondratschek, 1994), similar to its geometric meaning ['One must know the reference coordinate system ... Without this knowledge a geometric evaluation is impossible' (Wondratschek, 1994)]. For a wider functionality the concept of crystallographic symmetry matrix should be clarified.

The above remarks, and the fact that set $\mathbb{V}$ of 960 matrices with the determinant ± 1 and the elements of matrix powers $\{0, \pm 1\}$ covers arithmetic holohedries of Niggli-reduced cells (Lebedev *et al.*, 2006; Zwart *et al.*, 2006) as well as all Buerger-reduced highest-symmetry cells and their reciprocals (Stróż, 2011), suggest the possibility of constructing a finite, well defined arithmetic counterpart of Bravais lattices. Lattices related to less restrictive semi-reduced descriptions (s.r.d. lattices) or equivalently lattices with arithmetic holohedries describable in V should be more appropriate for symmetry analysis of primitive cells than strictly reduced lattices, since small deformations (phase transitions, experimental errors) do not need to be followed by discontinuous changes of lattice parameters.[1]

Having defined $\mathbb{V}$, the complete set of possible symmetry operations, its filtering according to an experimental s.r.d. metric should reveal all pseudo-symmetries. Ranking of the symmetry operations and in consequence ranking of the lattice types can be based on differences between the original and transformed lattice tensors (Macíček & Yordanov, 1992). However, these differences recalculated into cell deformations are better controlled by the precision of lattice measurement. Individual deformations can be used for estimation of the distance between the considered lattice and a lattice with strict symmetry [see extensive analysis of this problem in Andrews & Bernstein (2014) for Bravais symmetry determination and McGill *et al.* (2014) for database search].

2. Semi-reduction concept

If $A = [\mathbf{a}, \mathbf{b}, \mathbf{c}]$ defines a three-dimensional primitive lattice, then any $A' = Ag$, where $g \in GL(3, \mathbb{Z})$ describes the same lattice. The unique A' is constructed by lattice reduction procedures: $\mathbf{a}^2 + \mathbf{b}^2 + \mathbf{c}^2 = \min$ or $\mathbf{a}^2 + \mathbf{b}^2 + \mathbf{c}^2 + \mathbf{b} \cdot \mathbf{c} + \mathbf{a} \cdot \mathbf{c} + \mathbf{a} \cdot \mathbf{b} = \min$ and specific conditions, but the presence of experimental errors causes instability in the final conclusions.[2] In the simplified schemas a reduced cell is classified according to current metric relations, which is equivalent to rejection of other 'statistically' possible solutions. Thus, in the presence of experimental errors, we have two opposite demands: we must limit the variety of lattice descriptions like in the error-free case, but this limitation should not be too restrictive, since it leads to an artificial uniqueness and to rejection of alternative descriptions at a very early stage. This concept is well exposited in the statistical tests, where analysed models are frequently 'embedded' in a more general frame with a larger number of estimated parameters (Mandel, 1969).

[1] All the lattices given by the reduced tensor equation $(2, 2, 2, 0, 1, -1) + p(1, 0, 1, 0, 1, 0)$ differ only by the distance between planes perpendicular to the threefold axis, but this feature is difficult to recognize in three different Niggli-reduced cells, obtained for $p = 0$, $p < 0$ and $p > 0$. Such lattices are semi-reduced and border problems occurring in biased experimental data are inessential.

[2] For example, cubic primitive cell parameters with small random errors can mathematically suggest any crystallographic system (excluding a hexagonal one). Despite this, the cell shape and the lattice pseudo-symmetry will still be very close to a cube and the cubic system should be selected with some allowance for errors.

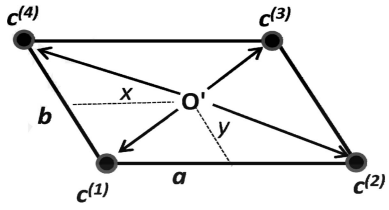


Figure 1
Four *semi-reduced* basis vectors $\mathbf{c}^{(n)}$ projected onto the upper plane nearest to the basis plane **ab**. Projected origin O is marked as O'.

The above demand leads to the introduction of *semi-reduced* basis vectors with the following geometric meaning. We consider one basis vector, say **c**, and a two-dimensional lattice described by shortest vectors **a** and **b**. The origin O projected orthogonally on the closest copy of the **ab** plane falls in the mesh cell at point O' in Fig. 1. Lattice points presented as solid circles, treated as the ends of vectors beginning at the origin, define four equivalent *semi-reduced* variants of given vector **c**.

Vector $\mathbf{OO'}$ orthogonal to **ab** can be reached from any vector $\mathbf{c}^{(n)}$ by a linear combination:

$$\mathbf{OO'} = \mathbf{c}^{(n)} + x_n\mathbf{a} + y_n\mathbf{b}. \tag{1}$$

Generally, there are four vectors $\mathbf{c}^{(n)}$, for which $|x_n| < 1$ and $|y_n| < 1$ are considered here as semi-reduced lattice vectors. If $|x_n|$ = min and $|y_n|$ = min or equivalently $|x_n|$, $|y_n| < 1/2$, $\mathbf{c}^{(n)}$ is simultaneously Buerger-reduced; if not it can be Delaunay-reduced. If $|x_n| = 1$ or $|y_n| = 1$, vector $\mathbf{c}^{(n)}$ is not semi-reduced, but can be Delaunay-reduced. If such a case occurs, there is also an equivalent Delaunay-reduced description with corresponding $|x_n| = 0$ or $|y_n| = 0$, which is semi-reduced, of course. The complete criterion can be based on a metric tensor in the symmetric or in the reduced form:

$$M = \begin{pmatrix} \boldsymbol{a}\cdot\boldsymbol{a} & \mathbf{a}\cdot\mathbf{b} & \mathbf{a}\cdot\mathbf{c} \\ \mathbf{b}\cdot\mathbf{a} & \mathbf{b}\cdot\mathbf{b} & \mathbf{b}\cdot\mathbf{c} \\ \mathbf{c}\cdot\mathbf{a} & \mathbf{c}\cdot\mathbf{b} & \mathbf{c}\cdot\mathbf{c} \end{pmatrix}$$

$$\text{or} \quad (\mathbf{a}\cdot\mathbf{a}, \mathbf{b}\cdot\mathbf{b}, \mathbf{c}\cdot\mathbf{c}, \mathbf{b}\cdot\mathbf{c}, \mathbf{a}\cdot\mathbf{c}, \mathbf{a}\cdot\mathbf{b}) \tag{2}$$

and its reciprocal

$$M^* = M^{-1}. \tag{3}$$

Criterion 1. A lattice is in s.r.d. if the moduli of off-diagonal elements in both the tensors M and M^{-1} are smaller than the corresponding diagonal elements sharing the same column or row:

$$|\mathbf{b}\cdot\mathbf{c}| < \mathbf{c}\cdot\mathbf{c}, \mathbf{b}\cdot\mathbf{b} \quad |\mathbf{a}\cdot\mathbf{c}| < \mathbf{c}\cdot\mathbf{c}, \mathbf{a}\cdot\mathbf{a} \quad |\mathbf{a}\cdot\mathbf{b}| < \mathbf{b}\cdot\mathbf{b}, \mathbf{a}\cdot\mathbf{a}$$

and simultaneously

$$|\mathbf{b}^*\cdot\mathbf{c}^*| < \mathbf{c}^*\cdot\mathbf{c}^*, \mathbf{b}^*\cdot\mathbf{b}^* \quad |\mathbf{a}^*\cdot\mathbf{c}^*| < \mathbf{c}^*\cdot\mathbf{c}^*, \mathbf{a}^*\cdot\mathbf{a}^*$$
$$|\mathbf{a}^*\cdot\mathbf{b}^*| < \mathbf{b}^*\cdot\mathbf{b}^*, \mathbf{a}^*\cdot\mathbf{a}^*. \tag{4}$$

Criterion 2. A lattice with symmetry describable in $\mathbb{V}$ is semi-reduced.

It is clear from Fig. 1 that all Buerger-reduced lattices and most Delaunay-reduced lattices are also in s.r.d. Since the semi-reduction is treated as a condition rather than as a reduction procedure, any lattice can be described in the s.r.d. form by the Buerger reduction procedure, without taking care of mathematical instabilities or multiple representations of a given lattice or also by the Delaunay reduction procedure after replacing some descriptions with equivalent but semi-reduced forms; for example the tensors (1, 2, 1, −1, 0, 0) and (1, 1, 1, 0, 0, 0) describe the same lattice, but only the latter one is in s.r.d. Because of the s.r.d. concept relations between arithmetic holohedries and lattice metrics are unbounded, not imposed by reduction criteria.

3. Affine symmetry matrices and their lattice context

A distance-preserving transformation called (linear) *isometry* or orthogonal transformation describes a proper or improper rotation. Without losing generality, in the Euclidean space represented by a Cartesian coordinate system, it takes the form of the orthogonal matrix

$$W(\alpha) = \pm\begin{bmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{5}$$

Determinant $\det(W) = \pm[\cos(\alpha)^2 + \sin(\alpha)^2] = \pm 1$, and thus each isometry is reversible. A reversal of W, that is rotation in the opposite direction, is equivalent to transposition, since $W^{-1} = W(-\alpha) = W^{\mathrm{T}}$. Another characteristic $\mathrm{tr}(W) = \det(W)[2\cos(\alpha) + 1]$ gives the information about the rotation angle. A composition of two orthogonal matrices results in a new orthogonal matrix; in consequence all such matrices constitute an infinite group of orthogonal matrices $O(3, \mathbb{R})$ with real entries. The group contains only 48 matrices with integer entries for $\alpha = 360/n$, n = 1, 2, 3, 4. Since *crystallographic restriction* also includes n = 6, symmetry of the hexagonal lattice cannot be described by orthogonal integer matrices.

In crystallographic coordinate systems imposed by lattice translation, symmetry matrices are frequently not orthogonal, but this inconvenience is outweighed by a simpler mathematics (W always contains integers) and closer relation with the corresponding lattice.

In passive interpretation, W transforms the lattice basis

$$A' = AW. \tag{6}$$

Taking into account the fact that the metric tensor

$$M = A^{\mathrm{T}}A \tag{7}$$

must be fixed, one can immediately obtain

$$M = A'^{\mathrm{T}}A' = W^{\mathrm{T}}MW. \tag{8}$$

By inverting (8) and with a little rearrangement we have an important property:

$$W^{-1} = M^{-1}W^{\mathrm{T}}M \tag{9}$$

Table 1
Complete set $\mathbb{M}$ of metrical tensors of highest-symmetry lattices referred to as semi-reduced bases.

Metrics *cI*5–*cI*16, reciprocal to *cF*5–*cF*16, describe non-Buerger cells (Stróż, 2011).

Lattice	Metric	Lattice	Metric	Lattice	Metric (*M*6)	Lattice	Metric
*hP*1	2,2,1,0,0,−1	*hP*4	2,2,1,0,0,1	*cF*7	2,2,2,0,−1,−1	*cI*7	4,3,3,1,2,2
*hP*2	2,1,2,0,−1,0	*hP*5	2,1,2,0,1,0	*cF*8	2,2,2,1,1,0	*cI*8	3,3,4,−2,−2,1
*hP*3	1,2,2,−1,0,0	*hP*6	1,2,2,1,0,0	*cF*9	2,2,2,1,0,1	*cI*9	3,4,3,−2,1,−2
cP	1,1,1,0,0,0			*cF*10	2,2,2,0,1,1	*cI*10	4,3,3,1,−2,−2
*cF*1	2,2,2,1,1,1	*cI*1	3,3,3,−1,−1,−1	*cF*11	2,2,2,1,−1,0	*cI*11	3,3,4,−2,2,−1
*cF*2	2,2,2,−1,−1,1	*cI*2	3,3,3,1,1,−1	*cF*12	2,2,2,1,0,−1	*cI*12	3,4,3,−2,−1,2
*cF*3	2,2,2,−1,1,−1	*cI*3	3,3,3,1,−1,1	*cF*13	2,2,2,0,1,−1	*cI*13	4,3,3,−1,−2,2
*cF*4	2,2,2,1,−1,−1	*cI*4	3,3,3,−1,1,1	*cF*14	2,2,2,−1,1,0	*cI*14	3,3,4,2,−2,−1
*cF*5	2,2,2,−1,−1,0	*cI*5	3,3,4,2,2,1	*cF*15	2,2,2,−1,0,1	*cI*15	3,4,3,2,−1,−2
*cF*6	2,2,2,−1,0,−1	*cI*6	3,4,3,2,1,2	*cF*16	2,2,2,0,−1,1	*cI*16	4,3,3,−1,2,−2

relating inversion and transposition of *W*. We can call *M* the *lattice context of W*.

The rightmost side of (8) due to (7) can be formally written as

$$(\mathbf{a}\cdot\mathbf{col}_1+\mathbf{b}\cdot\mathbf{col}_2+\mathbf{c}\cdot\mathbf{col}_3)(\mathbf{a}\cdot\mathbf{row}_1+\mathbf{b}\cdot\mathbf{row}_2+\mathbf{c}\cdot\mathbf{row}_3), \tag{10}$$

where vectors $\mathbf{col}_i$ and $\mathbf{row}_i$ symbolize the *i*th column and the *i*th row of *W*. By signed permutations of basis vectors one can obtain 48 basis variants (24 right- and 24 left-handed). Expression (10) is unchanged if such base variations are followed by *signed synchronous permutations* of rows and columns of *W*. This leads to up to 24 equivalent symmetry operations (or to the conjugacy class in group theory terms), if different.

We assign the name crystallographic symmetry matrix to any integer matrix *W* with det(*W*) = ±1 and a finite order (in group theory meaning); it does not matter if the lattice context is known or not. The matrix represents an isometric transformation in some coordinate system described by *M*, if *M* relates W^{-1} and transpose W^{T} by similarity equation (9). Such understanding of the symmetry matrix extends the set of 48 integer orthogonal matrices from a Cartesian system into an infinite set of matrices, which are also isometric operations, but in non-Cartesian systems (like the hexagonal one, or primitive). While finite order of *W* only 'promises' that a lattice exists with *W* as a symmetry operation, similarity equation (9) gives the possibility of finding the lattice. It can be noted that isometric transformations guarantee that any vector, including basis vectors, preserves its length. Generally, the fact that lengths of basis vectors before and after the transformation are unaltered is equivalent to the isometric property, but there are special lattices where it is not true (in some lattices several Buerger cells not related by symmetry can be selected).

A *holohedry*, a set of operations *W* which map any lattice onto itself in the isometric manner, is the finite subgroup of $GL(3;\mathbb{Z})$. It must contain elements *W* of finite order *k*, $W^k = I$, where *I* as usual denotes the identity matrix. The finite number of matrices can be obtained by limiting its elements, $\mathrm{abs}(W_{ij}) \leq m$, but more interesting is also extending this demand on W^k. For $m = 1$ there are 960 matrices organized in set $\mathbb{V}$ covered by the arithmetic holohedries of 39 highest-symmetry s.r.d. lattices (Table 1).

It is easy to conclude that all reduced metric tensors may be obtained from the four representatives *hP*1 (2, 2, 1, 0, 0, 1), *cP* (1, 1, 1, 0, 0, 0), *cF*1 (2, 2, 2, 1, 1, 1) and *cF*8 (2, 2, 2, 1, 1, 0) by composing two combinatorial operations: synchronous cyclic permutations of the diagonal and off-diagonal elements and multiplying any two off-diagonal items by −1. Finally, the obtained tensors should be doubled by a mathematical inversion and recalculated to integers. All tensors in Table 1 are semi-reduced.

Set $\mathbb{V}$ should be understood as some structure in $GL(3;\mathbb{Z})$ rather than as a set of loosely connected matrices (see the supporting information). Because of the comment to formula (10), it contains complete classes of orthogonally conjugated groups and in consequence orthogonal classes of individual matrices (maximum 24 long). The statistics of proper rotations are as follows: 81 (twofolds), 260 (threefolds), 126 (fourfolds), 12 (sixfolds) and of course one (identity operation). Derivation of a lattice context for any matrix from $\mathbb{V}$ is simple; in similarity equation (9) we are obligated to test only metric tensors from $\mathbb{M}$. If two symmetry matrices share the same lattice context (which is the rule for orthogonal matrices), their composition is also a symmetric matrix, otherwise not – the resulting matrix has an infinite order, even if it still represents isometric transformation. In every maximal group there are symmetry matrices characteristic for that group with the unique lattice context; other matrices are shared between two, three, four, five or 11 maximal groups.

4. Lattice orthogonalities

The classical symbol of a point (or space) symmetry operation (Fisher & Koch, 2006) originates from the linear algebra rather than from crystallography and describes the point-invariant subspace. Information on the complement subspace, invariant as a whole, is lost and the geometric sense of a symmetry matrix is treated as insignificant if the reference to the coordinate system is not known (Wondratschek, 1994).

In the crystallographic texts the symmetry of the arrangement of lattice points, and thus the derivation of the Bravais types, is explained geometrically by stacking identical plane lattices, relatively shifted one from another by some stacking vector (McKie & McKie, 1986). The generality will not be lost if we name the stack of planes by the Miller indices (*hkl*) and replace the stacking vector by the corresponding lattice direction [*uvw*]. A combined symbol [*uvw*](*hkl*) names the splitting of a three-dimensional lattice into the union of a two-dimensional lattice and a one-dimensional lattice. The splitting is orthogonal, if direction [*uvw*] is perpendicular to the plane family (*hkl*). Lattices can contain an infinite number of *general orthogonalities*; every direction [*uvw*] is perpendicular to the

Figure 2
Primary (empty) and secondary (filled) symmetry points on the lattice planes. The secondary symmetry points are seen in the conventional planar unit mesh to be 1/2, 0 or 0, 1/2, or 1/2, 1/2 for a twofold symmetry point, 2/3, 1/3 and 1/3, 2/3 for a threefold symmetry point, and 1/2, 1/2 for a fourfold symmetry point.

planes with the same Miller indices (uvw) in a cubic lattice, but we are interested in the *crystallographic orthogonalities* related to the lattice symmetry. In the following we will use the term *orthogonality* in this narrower sense. The limits of the dot product $[uvw]\cdot(hkl)$ for the odd and even symmetry axes were proved by Le Page (1982). The equality $uh + vk + wl = 1$ means that the lattice is primitive in direction $[uvw]$ and a symmetry axis consists of the primary symmetry points (Fig. 2) in the stacking sequence of planes (hkl). If the dot product is equal to 2, a twofold or a fourfold symmetry axis intersects alternately the family planes (hkl) in primary and secondary symmetry points. For the dot product equal to 3, possible only for a threefold symmetry axis, this sequence is 'primary, secondary, secondary, primary, secondary, . . .'.

The number of orthogonalities classifies the crystallographic systems in order of decreasing symmetry: 13 – cubic, 7 – hexagonal, 5 – tetragonal, 4 – trigonal (rhombohedral), 3 – rhombic, 1 – monoclinic and 0 – triclinic. Orthogonalities in the reciprocal lattice remain, but with interchanged indices $[hkl](uvw)$. The task of finding all orthogonalities for lattices in s.r.d. can be treated as solved. Matrices in $\mathbb{V}$ are enumerated and a new geometric symbol n^{+-} $[uvw](hkl)$ (Stróż, 2011) for a symmetry matrix explicitly contains the orthogonality description (see the supporting information). We distinguished 208 orthogonalities; some are well known from the conventional lattice descriptions, 81 concerning twofolds were earlier enumerated (Zwart *et al.*, 2006).

Some properties of $[hkl][uvw]$ are mathematically obvious; it specifies two parallel directions, in direct and reciprocal spaces. The orthogonalities can be roughly grouped by a parameter

$$\cos^2\delta = \frac{(uh + vk + wl)^2}{(uu + vv + ww)(hh + kk + ll)}. \qquad (11)$$

In s.r.d. there are only six different $\cos^2\delta$ values: 1, 2/3, 3/4, 4/5, 9/11, 9/14, and thus six groups of splitting indices.[3] But such formal grouping has little meaning and the equivalence classes can be obtained by further subdivision of the group '1' and '2/3'. These lead to nine types of orthogonalities (Fig. 3).

Two different cases can be easily recognized. In the first configuration, one basis vector agrees, and the two remaining are perpendicular to the lattice vector invariant under the symmetry operation. This situation, presented in the leftmost

[3] Group '1/2' should be added to this compilation if we also take into account orthogonalities in Delaunay-reduced cells.

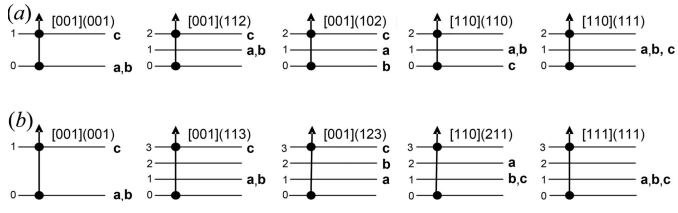


Figure 3
Orthogonality types in s.r.d. Only one interpretation is presented: symmetry axes are parallel to $[uvw]$, basis vectors end in levels h, k, l of the family of lattice planes (hkl). Sketches (a) and (b) show the splitting indices, which correspond to the action of even-order and threefold rotation axes, respectively.

pictures of the rows (a) and (b) in Fig. 3, is compatible with all types of symmetry axes. The lattice is primitive in the axis direction, since dot product $[uvw]\cdot(hkl) = 1$.

In the remaining configurations, one, two or even all basis vectors are inclined to the invariant direction. This corresponds to the centred Bravais cells. The compatibility with the even-order rotation axis or threefold rotation axis is determined by the dot product equal to 2 or 3, respectively.

Splitting indices $[uvw](hkl)$ extract the lattice orthogonalities hidden in the metric tensors as well as in the arithmetic holohedries. The angle between two symmetry axes given by $[u_1v_1w_1](h_1k_1l_1)$ and $[u_2v_2w_2](h_2k_2l_2)$ can be calculated from the indices themselves:

$$\cos^2\varphi = \frac{\{[u_1v_1w_1]\cdot(h_2k_2l_2)\}\{[u_2v_2w_2]\cdot(h_1k_1l_1)\}}{\{[u_1v_1w_1]\cdot(h_1k_1l_1)\}\{[u_2v_2w_2]\cdot(h_2k_2l_2)\}}. \qquad (12)$$

The derivation of angles between symmetry elements in a cubic system is given in §*A*1.

Thus, symmetry visualized by Bravais lattices is also seen in s.r.d. lattices *via* orthogonalities. Although arithmetic groups depend on the basis selection, the space distribution of orthogonalities is completely coordinate-free and represents the whole lattice rather than its primitive cell.

5. Critical lattice deformations and derivative lattices

The treatment of lattice deformations in accordance with the group–subgroup chain of resulting holohedries is facilitated by selecting $[UVW](HKL)$ and analysing possible deformations of $\mathbb{M}$, in such a way that the given orthogonality remains and the lattice symmetry is unchanged or lowered. Assuming only proper rotations, in all cases the final lattice group should be 2 or 32 depending on the dot product $[UVW]\cdot(HKL)$ (see Fig. 3). It will be adequate for our purpose to consider only a homogeneous stretching or a compressive deformation of the interplanar distance $d_{(hkl)}$. The resulting *deformation tensor* $\varepsilon d_{(hkl)}$ is symmetric and can be presented in the reduced form:

$$\varepsilon d_{(hkl)} = \Delta M = \varepsilon(hh, kk, ll, kl, hl, hk). \qquad (13)$$

A deformation which lowers the lattice symmetry is *critical*, otherwise not. It is obvious that deformation $\varepsilon d_{(hkl)}$ retains orthogonalities (if any) with direction $[uvw]$ perpendicular or parallel to the (hkl) plane and destroys others. For a selected

Table 2
Hierarchy of spaces with invariant linear transformations: projective, affine, Euclidean and crystallographic [the latter is represented by semi-reduced descriptions (s.r.d.)].

Legend: *GL* and *O* – general and orthogonal matrix groups with real ($\mathbb{R}$) or integer ($\mathbb{Z}$) elements, *I* – identity matrix.

Space	Group element, **W**	Linear transformation	Invariant features
Projective space	$\mathrm{Det}(\mathbf{W}) = 0$	Projection, non-reversible	Cross ratio
Affine space – no metric	$\mathbf{W} \in GL(3,\mathbb{R})$, $\det(\mathbf{W}) \neq 0$	Affine transformation	+ Linearity
Euclidean space – Euclidean metric, *I*	$\mathbf{W} \in O(3,\mathbb{R})$, $\det(\mathbf{W}) = \pm 1$	Isometry	+ Distances
Crystallographic space (s.r.d.)	$\mathbf{W} \in GL(3,\mathbb{Z})$ and $\mathbf{W}^k = I$	Crystallogaphic operation	+ Orthogonality; nine types
– derivative of 39 metric types	960 **W**, $\det(\mathbf{W}) = \pm 1, \mathbf{W}_{ij} = \{-1,0,1\}$		

orthogonality $[UVW](HKL)$ up to three critical deformations can be constructed. This list is amended by scaling distortion, which never is critical.

(*a*) Distortion $pd_{(HKL)}$. This vertical deformation can be critical only for highest-symmetry lattices, where orthogonalities inclined to the selected one may exist. Metrical relationships on plane (HKL) are not changed.

(*b*) Distortion $qd_{(hkl)}$. Horizontal distortion $qd_{(hkl)}$ is not unique, but limited to twofold operations $2[uvw](hkl)$, where $(hkl)\cdot(UVW) = 0$. It modifies the metrical relationships between two orthogonal lattice vectors on the plane (HKL) and is critical if the plane symmetry is changed.

(*c*) Distortion $rd_{(h'k'l')}$. This horizontal deformation is completely arbitrary, but still $(h'k'l')\cdot(UVW) = 0$. It destroys all lattice orthogonalities in the plane (HKL).

(*d*) Distortion sM. This deformation proportionally changes the lattice metric, not its symmetry.

Lattices obtained by the above distortions are derivative according to highest-symmetry lattices in $\mathbb{M}$.

Lemma. The symmetry of derivative lattices in s.r.d. covers all arithmetic holohedries in $\mathbb{V}$.

Proof. Arithmetic holohedries of maximal symmetry lattices $M \in \mathbb{M}$ can be obtained and geometrically interpreted by filtering matrices from $\mathbb{V}$. Each orthogonality $[UVW](HKL)$ defines one (or a few) group–subgroup chain(s) and corresponding deformations retaining this orthogonality. Derivative lattices are still in s.r.d. and their successive metrics are as follows:

$$
\begin{aligned}
&M,\\
&M(p) = M + pd_{(HKL)},\\
&M(p,q) = M(p) + qd_{(hkl)}\\
&\ldots \text{All possible variants of twofolds}\\
&M(p,q,r) = M(p,q) + rd_{(h'k'l')},\\
&M(p,q,r,s) = M(p,q,r) + sM.
\end{aligned}
$$

Theoretically, all non-triclinic lattices in s.r.d. are describable by the metric M from $\mathbb{M}$. Thus, $\mathbb{M}(p,q,r,s)$ symbolizes all derivative lattices, a specific $M(p,q,r,s)$ characterizes the given holohedry. An infinite number of three-dimensional lattices with non-triclinic symmetry can be derived from a finite number of highest-symmetry lattices by a well defined procedure of breaking symmetry. Since deformations are limited to changing interplanar distances, this formalism seems to be helpful in X-ray powder diffraction analysis of structural phase transitions (see illustrative §*A*2). □

6. Crystallographic space in semi-reduced description

The essence of the famous Erlangen program (Klein, 1872) consists of a unified way of hierarchical classification of geometries (spaces) based on the group–subgroup relations between the corresponding groups of transformations, invariant in given geometries. In particular, the projective geometry is less restrictive than the affine geometry, which in turn is less restrictive than the Euclidean geometry.

The crystallographic geometry, limited to the geometry and symmetry of Bravais cells, is typically interpreted as a special case of Euclidean geometry (Kopský, 2001), with the individual treatment of the hexagonal system. Such an elegant approach has many advantages: (i) the relation between parameters of a Bravais cell and its symmetry is obvious, (ii) the number of symmetry matrices is limited to 48 orthogonal matrices with integer elements (+ 16 non-orthogonal matrices for the hexagonal system), (iii) symmetry matrices are simple, only three matrix elements differ from zero (four for the hexagonal system). This is the reason why Bravais cells stand for a conventional space-group characterization and in consequence for a standardized crystal structure description.

For many practical problems the crystallographic geometry should be analysed in its own non-Cartesian systems. While Bravais lattices can be relatively well described in a three-dimensional Euclidean space, dealing with the symmetry of reduced cells will be possible in the union of linear subspaces of six-dimensional (or five-dimensional) parametric space. Typically, such spaces are partial, restricted by the mathematical reduction theory. Considerations presented in preceding paragraphs showed a possibility of formally introducing a more complete crystallographic space, limited by the lattice geometry in s.r.d. This provides a better conceptual and practical framework for dealing with the symmetry of reduced lattices also in the presence of experimental errors or deformations. The lattice geometry being more specialized in comparison with the Euclidean geometry can be considered as a separate item in the hierarchy of spaces with invariant linear transformations (Table 2).

Table 3
The distribution of arithmetic holohedries in s.r.d. along the Bravais types.

Type	*hP*	*cP*	*cF*	*cI*	*tP*	*tI*	*oP*	*oA*	*oI*	*oF*	*hR*	*mP*	*mC*	*aP*†
No	6	1	16	16	3	60	1	15	28	28	124	3	78	1

† Anorthic lattices are not considered in s.r.d. space.

The properties of hierarchical spaces (projective, affine, Euclidean) are discussed elsewhere. We recall here only some features. A linear transformation in the *projective space* reduces the dimension of that space and can retain the ratio of ratios (cross ratio) on a line. Such transformations are not invertible. The operations in the *affine space* are any linear transformations that do not change the space dimension: W belongs to a general linear group $GL(3, \mathbb{R})$. The *Euclidean space* is an affine space equipped with the Euclidean metric tensor $M = I$, where I denotes the *identity* matrix. The Euclidean operations called isometries are distance-preserving mappings and thus retain distances. For the crystallographic space treated as a special type of Euclidean space, additional requirements on W are needed. Such an approach is applicable for lattice description by the Bravais cells, with some problems involving the hexagonal system.

In the *crystallographic space* the set of operations that map any lattice onto itself in the orthogonal manner is a finite subgroup of $GL(3, \mathbb{Z})$. Finite subgroups contain elements W of finite order k, $\mathbf{W}^k = I$. In $GL(3, \mathbb{Z})$ the k may only take values 1, 2, 3, 4, 6 and thus the 'crystallographic restriction' has a natural origin. $GL(3, \mathbb{Z})$ can be well represented by $\mathbb{V}$ in s.r.d. approximation.

7. Isometries in the presence of experimental errors

Two aspects should be taken into account while deriving the arithmetic holohedry from the biased data. At first, the process is not algorithmic; mathematically, it can be recognized as a Diophantine problem, computationally, as a *brute force* approach, *e.g.* filtering of all potential solutions. Secondly, there is no internal criterion to decide whether some deviations from an isometric operation are essential for the symmetry recognition or are accidental.

The filtering process (9) is extremely simple: only two multiplications of matrices and comparison of the resulting metric tensor with the original one for each $V \in \mathbb{V}$. Comparison made on cell parameters (14) controls independently deviations from isometric and isogonal transformations. Moreover, the deviation δ (Le Page, 1982) from orthogonality between $[uvw]$ and (hkl) can be monitored. Two filter parameters are introduced: tol1, allowable relative cell-length changes given in per cent; and tol2, an allowable change of the cell angles given in degrees of arc. The same numerical order of both tolerances is assumed. Comparable cell parameters are given by the following scheme:

$$a, b, c, \alpha, \beta, \gamma \rightarrow M \rightarrow V^{\mathrm{T}}MV = M' \rightarrow a', b', c', \alpha', \beta', \gamma'. \quad (14)$$

Finally, the filtering criterion is described by inequalities:

$$\Delta a = 100 \times \max\left(\frac{|a' - a|}{a}, \frac{|b' - b|}{b}, \frac{|c' - c|}{c}\right) < \mathrm{tol1}(\%), \quad (15)$$

$$\Delta\alpha = \max(|\alpha' - \alpha|, |\beta' - \beta|, |\gamma' - \gamma|, \delta) < \mathrm{tol2}(^\circ). \quad (16)$$

Both tolerances are symmetry thresholds for ranked isometric and isogonal transformations. Their values are related to the experimental standard deviations, but can be reduced to zero for modelled strict symmetry data or enlarged for highly corrupted data. Moreover, if we release tol2 and the filtering procedure finds some additional matrices in $\mathbb{V}$ with high angular discrepancies, it will be evident that the lattice also reveals two-dimensional symmetry[4] characteristic of multiple Buerger-reduced cells. If tolerances are relatively high (*e.g.* tol1 = tol2 = 3, see §*A*3 and Le Page arguments for selecting such a high level) this measure is mathematically stable. Small changes in the input cell parameters will result in modifications of discrepancies, but not in the list of filtered pseudo-symmetry matrices and in consequence in the pseudo-symmetry of the lattice. If $\max(\Delta a)$ and $\max(\Delta\alpha)$ may be accepted by the experimental precision, the pseudo-symmetry group represents the lattice symmetry. Any subgroup of such a maximal group is also compatible with the given metric, like in strict symmetry cases, but is less important for recognition of the Bravais type (§*A*3).

Generally, the results of matrix filtration can be understood as a complex geometric description of lattice isometries in the presence of controlled experimental errors.

8. Semi-reduced lattice types

In sharp contrast to the *uniqueness* of lattice classification by reduced cells, splitting semi-reduced lattices by their holohedries is not lattice classification, but due to the *completeness* in $\mathbb{V}$ it simplifies and stabilizes such a process. The distribution of arithmetic holohedries along the Bravais types (Table 3) was obtained by generating derivative lattices $\mathbb{M}(p, q, r)$. Some results were confirmed by analysis of geometric interpretation of matrices in $\mathbb{V}$; among 126 fourfold operations 120 are centred (= 60 *tI* groups). Similarly, centring takes place for 248

[4] In this context matrix V describes an *isometric transformation limited to basis vectors*. It is not an orthogonal transformation; angles and other distances are changed.

threefolds (= 124 *hR* groups) from the complete set of 260 items, 78 twofolds are centred (= 78 *mC*) and three are not (= 3 *mP*). This gives 379 primitive lattice types.

The number of semi-reduced types increases about nine times in comparison with 44 Niggli characters, but criteria for each type do not need to be given explicitly, since there is one-to-one correspondence between an s.r.d. type and its symmetry (individual arithmetic holohedry). Thus all levels of lattice characterization are consistent and complete in $\mathbb{V}$: crystallographic systems – all geometric holohedries, Bravais types – all geometric holohedries + all centring modes, s.r.d. types – all arithmetic holohedries.

9. Discussion

About 75% of known crystalline materials belong to the non-triclinic systems, which is many orders higher than the estimation based on a random distribution of cell parameters. However, symmetry (the possibility of equivalent lattice descriptions) contrasts with the uniqueness of lattice definition. From the symmetry point of view the unique classification of reduced lattice descriptions is an artificial step which in the presence of experimental errors leads to unnecessary mathematical instabilities. Alternative stable techniques, based on a *brute force* strategy, can be effective if the set of potential solutions is not considerable. Such a requirement was fulfilled by the Le Page method, but innovative concepts contained therein were not generally appreciated.[5] The idea of finding lattice symmetry by searching a spatial distribution of all possible twofold axes (and thus lattice orthogonalities) was extended in the present work to filtering possible symmetry matrices according to the lattice metrics. This eliminates the necessity of the arithmetic holohedry construction. The goal was achieved – analysis of symmetry changes on the arithmetic level, without relations to Niggli or conventional cells. Moreover, the simplicity of the filtration method seems to be an interesting step in building a full computer program for automatic Bravais-lattice selection from the experimental cell with controlled standard errors, relatively simple in comparison to the existing ones. Since similar lattices differ only by small deformations, they must share the same pseudo-symmetry, even if the strict lattice symmetries are lower. The filtering procedure is resistant against extra two-dimensional symmetries, which are not three-dimensional symmetries. However, these two-dimensional symmetries lead to multiple Buerger-reduced cells (Gruber, 1973) and complicate Niggli-cell selection. Ranking of individual operations helps in distinguishing between 'random' and 'systematic' lattice distortions. For example, similar deviations caused by all threefold operations cannot be interpreted as rhombohedral distortion of a cubic cell, even if a *hR* lattice is usually reported as possible symmetry in biased cubic cells. However, if it is possible to split filtered operations into two separate parts (*hR* group and the rest of the operations) by selecting appropriate thresholds tol1 and tol2, the rhombohedral distortion cannot be interpreted as accidental.

Splitting indices derived from the symmetry matrices in $\mathbb{V}$ describe a complete set of orthogonalities. Potential orthogonalities occurring in the semi-reduced lattice tensors can be generated according to the orthogonality types and combinatorial rules. It is not surprising. In enumerative combinatorics, many of the problems that arise in applications have a relatively simple combinatorial description, if they are 'complete' relative to some requirements. Arithmetic holohedries of reduced lattices do not constitute complete sets, which is opposite to the proposed semi-reduced lattice descriptions: $\mathbb{V}$ – all symmetry matrices with elements $\{-1, 0, 1\}$, $\mathbb{M}$ – all maximal groups in V, $\mathbb{M}(p, q, r)$ – all s.r.d. classes or all arithmetic holohedries in $\mathbb{V}$. Completeness of the semi-reduced lattice space reveals well its internal and combinatorial structure and simplifies rather than complicates relations between a lattice metric and the symmetry. Set $\mathbb{M}$ may be obtained from the four representatives *hP*1, *cP*, *cF*1 and *cF*8. For $\mathbb{V}$ generation, only 11 symmetry matrices are necessary. All three levels of lattice classifications are complete and consistent in $\mathbb{V}$: crystallographic systems – all geometric fingerprints of holohedries, Bravais types – all system holohedries + all centring modes, primitive lattice types – all individual arithmetic holohedries. Since representatives *hP*1, *cP*, *cF*1 and *cF*8 correspond to generators selected by Hosoya (2000), for derivation of the unified group of all the Bravais lattices G_0, it is possible that some properties of $\mathbb{V}$ can be explained in terms of this huge (2 799 360 elements) group.

Matrices $V \in \mathbb{V}$ are natural extensions of 48 orthogonal integer matrices and 16 orthogonal non-integer ones (hexagonal system), if the equality $V^{-1} = V^{\mathrm{T}}$ will be replaced by the similarity operation $V^{-1} = M^{-1}V^{\mathrm{T}}M$, where the symmetrical positively defined matrix M gives the lattice context.

In the proposed crystallographic space the geometric meaning of V, based on splitting indices, plays a fundamental role. Dual symbols allow deduction of transformation to the Bravais lattice, classification of arithmetic holohedries on the absolute basis, classification of crystallographic orthogonalities, analysis of the lattice deformations and estimation of the length of an orthogonal conjugacy class. Moreover, splitting indices give the lattice context of a symmetry operation or a symmetry element, where they may be compared with the concept of 'geometric element' (de Wolff *et al.*, 1989). In the case of space-group operations, it allows returning to the earlier definition of symmetry elements based on cyclic subgroups (Stróż, 2012).

10. Summary

By composing a few crystallographic concepts with partial data concerning arithmetic holohedries into a complete system, a more convenient framework to study symmetry changes of deformable lattices was developed. It extends obvious relationships between cell shapes, symmetry elements, symmetry matrices and simple deformations, from the centred

[5] 'The method seems only to be suited to Bravais lattices determination' (Andrews & Bernstein, 1988).

Table 4
Space distribution of symmetry axes in the cubic system.

Interaxial angles were derived from the arithmetic holohedry itself, without any metrical data.

	2	3	4	5	6	7	8	9	10	11	12	13
1	90	90	54.74	54.74	54.74	54.74	45	45	90	45	45	90
2		90	54.74	54.74	54.74	54.74	45	90	45	45	90	45
3			54.74	54.74	54.74	54.74	90	45	45	90	45	45
4				70.53	70.53	70.53	90	35.26	35.26	35.26	90	90
5					70.53	70.53	35.26	90	35.26	90	35.26	90
6						70.53	35.26	35.26	90	90	90	35.26
7							90	90	90	35.26	35.26	35.26
8								60	60	90	60	60
9									60	60	90	60
10										60	60	90
11											60	60
12												60

Bravais lattices to a wide class of primitive lattices. A simple filtering of well defined symmetry matrices according to the biased experimental metric leads to a rich and mathematically stable characterization of a lattice in the form of ranked deviations from the orthogonalities, isometric and isogonal transformations. Metrical symmetry corresponds to the maximal arithmetic group of pseudo-symmetries allowed by estimated or assumed tolerances: tol1, tol2. Geometric interpretation of filtered matrices defines transition to the Bravais cell. All subgroups of the pseudo-symmetry group are consistent with given lattice data, but the most important are subgroups obtainable by limiting tol1 and tol2. In the presence of experimental errors, filtering of symmetry matrices avoids missing important candidates for the lattice types, without excessively producing all mathematically possible lattices with lower symmetries.

'Lattice similarities' is rather a side problem in the scope of this work, but very important for practical crystallography and database searching. In the presented approach the similar lattices are such lattices that share the pseudo-symmetry lattice type and reveal similar Bravais cell parameters (both in given limits tol1, tol2). Preliminary comparison of this criterion with the distance measure based on careful analysis of the Niggli reduction boundaries (Andrews & Bernstein, 2014) was promising. Extensive comparison of such different concepts should be interesting and valuable.

It is clear that the numbers of different objects (symmetry matrices, directions, elements *etc.*) related to lattices in s.r.d. are higher than the numbers of analogous objects related to strictly reduced lattices, but completeness of the semi-reduced lattice space reveals its combinatorial structure, which is eminently more suitable for computer applications than restrictive rules specific rather for the reduction process than for lattices themselves. It can be finally concluded that there are excellent theoretical and practical reasons (including stability, simple mathematics and algorithms) for looking at the strict or distorted crystal lattice symmetry from an entirely new and surprising point of view – the combinatorial set $\mathbb{V}$ of matrices, their semi-reduced lattice context and their geometric properties.

APPENDIX *A*

A1. Example 1. Geometric fingerprints of holohedries

All conjugate arithmetic holohedries and the corresponding geometric holohedry share the same geometric fingerprint – the space distribution of symmetry axes. For derivation of interaxial angles we do not need metrical information, but only dual indices (10).

Let us enumerate symmetry elements of the *F*-centred cubic lattice in *cF*5 description: 1: 4[112](001), 2: 4[$1\bar{1}0$]($1\bar{1}0$), 3: 4(110)[$11\bar{1}$], 4: 3[$\bar{1}1\bar{2}$]($01\bar{1}$), 5: 3[132](010), 6: 3[$\bar{1}12$]($\bar{1}01$), 7: 3[312](100), 8: [011]($\bar{1}11$), 9: [001]($\bar{1}\bar{1}2$), 10: [010]($02\bar{1}$), 11: [101]($1\bar{1}1$), 12: [111](110) and 13: [100]($20\bar{1}$). Twofold axis symbols are omitted from items in the list. The space distribution of symmetry elements, according to the given numbering, is compiled in Table 4.

The same results, up to ordering schema, can be obtained for the rest of the 32 holohedries of cubic lattices described in Table 1. Similarly, six holohedries corresponding to the lattice metrics *hP*1–*hP*6 gave the space distribution of symmetry elements characteristic for the hexagonal system. Thus, all matrices in *V* (excluding only the identity matrix) are involved with two geometric structures.

A2. Example 2. Modelling of the *S*-phase cell

The hardness and the wear resistance of austenitic stainless steel are improved by a surface treatment. Special nitriding processes lead to super-saturated layers (*S*-phase); the formation, structure and dependence on the nitrogen amount are still not fully understood (Fewell *et al.*, 2000).

X-ray powder diffraction experiments (Fig. 4) showed an apparent contradiction between a non-homogeneous reflection shift (breaking symmetry) and the lack of splitting diffraction lines characteristic for such cases. This caused problems in an automatic cell derivation. Since the unit cell expands and the smallest deformation occurs for (111) interplanar spacings, the *S*-phase metric can be modelled by

$$M_{S\text{-phase}} = M_{\text{austenite}} + sM_{\text{austenite}} + p(1, 1, 1, 1, 1, 1).$$

Table 5
Numerical experimental data for interplanar distances.

Differences in *d*-spacings suggest rhombohedral distortion of the austenite cubic cell.

Miller indices (*hkl*)	Interplanar distance $d_{(hkl)}$ (Å)			
	Austenite	*S*-phase (experimental)	*S*-phase (model)	Error (%)
(111)	2.080	2.254	2.254	0.0
(200)	1.800	2.009	2.010	0.0
(220)	1.270	1.402	1.400	−0.1
(311)	1.083	1.191	1.189	−0.1
(222)	1.037	1.125	1.127	0.2
(400)	0.900	1.004	1.004	0.1

Table 6
Complex characterization of the metric symmetry of the lattice in the presence of experimental errors.

The assessment of the arithmetic holohedry depends on acceptable tolerances.

No.	Δa (%)	$\Delta\alpha$ (°)	δ (°)	Dual symbol
1	0.000	0.000	0.000	1 [] ()
2	0.006	0.007	0.005	2 [$\bar{1}$02] (001)
3	0.998	1.145	0.714	2 [$\bar{1}$20] (010)
4	0.998	1.145	0.714	2 [100] (211)
5	2.482	1.125	0.714	4^+ [100] (211)
6	2.488	0.027	0.714	4^- [100] (211)
7	2.482	0.020	1.480	2 [01$\bar{1}$] (01$\bar{1}$)
8	2.488	1.125	1.482	2 [$\bar{1}$11] (011)

Parameters *p* and *s* estimated by the least-square method explain the behaviour of *S*-phase reflections (Table 5). The lack of splitting lines can be easily explained by the texture: the deformation occurs only in the [111] direction closest to the direction of nitrogen impacts, normal to the sample surface.

A3. Example 3. Bravais-lattice determination from the arithmetic holohedries

A semi-reduced cell is given by the parameters $a = 4.000$, $b = 4.472$, $c = 4.583$ Å, $\alpha = 79.030$, $\beta = 64.130$, $\gamma = 64.150°$ (Le Page, 1982). High thresholds (tol1 = 3%, tol2 = 3°) were selected for filtering matrices (Table 6).

The estimated holohedry corresponds to the lattice type *tI*. If the cell parameters are measured with higher precision estimated by tol1 = 1 and tol2 = 1.5, only the first four rows describe the symmetry operations and the holohedry is *oF*. If we know that the lattice metric was obtained by very precise measurements (modelled by tol1, tol2 = 0.01), the real symmetry cannot be higher than *mC*. These maximal symmetries are 'suggested' by deviations Δa, $\Delta\alpha$, δ. Of course, other subgroups of *tI* are consistent with the given lattice data, but are less important for selection of the Bravais cell, that is the cell that corresponds to the highest lattice symmetry in known or assumed error limits.

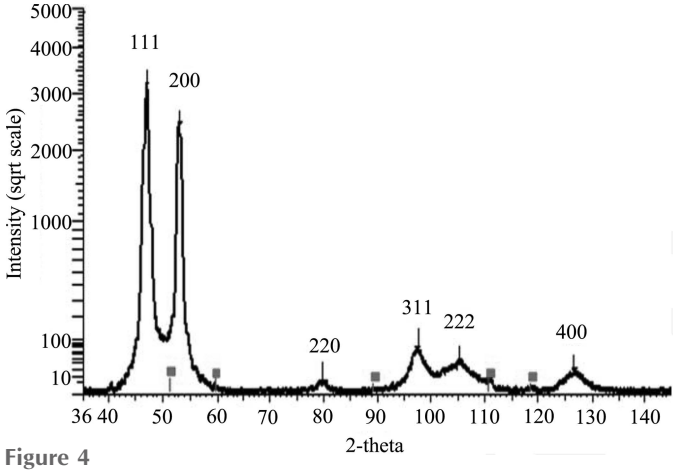


Figure 4
Diffraction pattern of the *S*-phase (deformed austenite) caused by plasma nitridation (Stróż & Psoda, 2010). Markers show original austenite reflections.

The above results agree with the output of Le Page's program from 1982. Comparison with 'metrical' programs should be preceded by analysis of the cut-off criteria of both approaches. As an *ad hoc* solution of this problem, 'metrical' results may be checked for accordance with selected symmetry tolerances. Such exemplary data are collected in Table 7.

The filtering procedure for Niggli-reduced cells from Table 7 reveals symmetry described in the last column for tol1, tol2 $\simeq 0$. But all lattices in ranges tol1, tol2 = 3 show *tI* pseudo-symmetry, in contrast to other Bravais lattices rejected by this *ad hoc* rule. The pseudo-symmetry and the exact symmetry are in a group–subgroup relation. Such 'structural transitions' can be modelled by deforming the lattice with strict *tI* symmetry. For example, one can obtain an *mC* lattice (3.986, 8.1591, 4.528, 90, 116.039, 90), the Niggli-reduced form of which reveals a 2 [$\bar{1}$02] (001) symmetry operation and *tI* pseudo-symmetry. Such a lattice is closer to experimental data in comparison with the lattice (4.123, 8.186, 4.243, 90, 116.481, 90) obtained by *BGAOL* but not included in Table 7, since it reveals *mC* symmetry; however, it does not reveal tetragonal pseudo-symmetry for given tolerances.

It is clear from the above comparison that pseudo-symmetry is a valuable measure of similarities between lattices, even in the vicinity of 90° angles. In the presence of experimental errors, filtering of symmetry matrices $\mathbb{V}$ avoids missing important candidates for the lattice types, without excessively producing all mathematically possible lattices with lower symmetry.

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Table 7
Bravais items from *BGAOL* output (http://iterate.sf.net/bgaol), which corresponds to pseudo-symmetry *tI* for tolerances tol1, tol2 = 3.

a	*b*	*c*	α	β	γ	Symmetry
5.752	5.752	3.981	90	90	90	*tI*
8.009	8.257	3.981	90	90	90	*oF*
3.983	5.739	5.762	90	90	90	*oI*
6.986	5.762	4	90	124.427	90	*mC*
4	8.247	4.472	90	115.852	90	*mC*
3.975	8.012	4.583	90	115.907	90	*mC*
5.762	3.983	5.739	90	91.742	90	*mI*

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