SYMMETRY OF CRYSTALLINE STRUCTURES
A new look at it, motivated by the study of phase transformations in crystals

Mario Pitteri (with Giovanni Zanzotto)
DMMMSA-Università di Padova
Via Belzoni, 7, 35131 PADOVA ITALY
pitteri@dmsa.unipd.it

1. CRYSTALLINE STRUCTURES
Consider first the simplest triply-periodic structures, that is, simple lattices (or 1-lattices):
\[ \mathcal{L} = \{ N^a e_a, a = 1, 2, 3, N^a \in \mathbb{Z} \} = \mathcal{L}(e_a). \]

The lattice vectors \( e_a \) (also called the lattice basis) are linearly independent.

While the lattice basis \( e_a \) uniquely determines the 1-lattice \( \mathcal{L}(e_a) \), the converse does not hold:
\[ \mathcal{L}(\vec{e}_a) = \mathcal{L}(e_a) \iff \vec{e}_a = m^b_a e_b, \quad m \in GL(3, \mathbb{Z}) \tag{1} \]
(in the 2-d case, \( m \in GL(2, \mathbb{Z}) \)). Here \( GL(3, \mathbb{Z}) \) is the group of 3 by 3 integral matrices with determinant \( \pm 1 \), with the obvious analogue for \( GL(2, \mathbb{Z}) \).

Real crystals are not in general 1-lattices. We need multilattices, which are union of \( n \) interpenetrating translates of a 1-lattice. A simple, well known example is the hexagonal close-packed structure:
2. ‘GEOMETRIC’ SYMMETRY OF SIMPLE LATTICES

In the study of crystal symmetry various aspects have been considered classically: KEPLER (1611-1619), followed by HOOKE (1665) and, later, HA Õ Y (1822), studied periodic structures, and tiling and packing problems.

A major early advance was the classification of the different ‘kinds’ of subgroups of $O(3)$, by various authors, circa 1830. These are the famous ‘point groups’, that is, the groups of symmetries of bounded objects. The name relates to the fact that any affine isometry leaving a bounded object invariant has a fixed point.

Here, ‘kind’ means conjugacy class in $O(3)$. This criterion is motivated by the idea that ‘rotated’ objects are regarded to have essentially the same symmetry.

Disregarding the cases of isotropy (sphere) and transverse isotropy (circular cylinder), and considering only the proper orthogonal transformations, we have:

THEOREM: The finite subgroups of $SO(3)$ (rotations) are all orthogonally equivalent to a group in the following list:

$$1, \ Z_n, \ D_n, \ T, \ O, \ I.$$ 

These are respectively the symmetry groups of an asymmetric body, of the n-pyramid, of the n-prism, and of the five Platonic solids: the tetrahedron, the octahedron (and the cube), and the icosahedron (as well as the dodecahedron).

When also $-1$ is taken into account, the situation is slightly more complicated. The possible groups are obtained by suitably ‘patching together’ subgroups of the groups above, possibly multiplied by $-1$. An important COROLLARY is the following:

Among the above infinite ones, 32 are the classes (‘crystal classes’) of groups that leave some simple lattice invariant; their elements satisfy the ‘crystallographic restriction’: their order can only be 1, 2, 3, 4 or 6. Groups belonging to these 32 crystal classes are called crystallographic point groups.

The (crystallographic) point group, $P(e_a)$, of the lattice $L(e_a)$ is thus defined as:

$$P(e_a) = \{Q \in O(3) : QL(e_a) = L(e_a)\}. \quad (2)$$

Hence, by (1), $Q \in O(3)$ belongs to $P(e_a)$ if and only if there is $m \in GL(3, \mathbb{Z})$ such that

$$Qe_a = m_a^b e_b. \quad (3)$$

Only the groups in 7 among the 32 crystal classes are maximal for the property of leaving a 1-lattice invariant; these are called the crystal systems, with the familiar names:

Triclinic, monoclinic, orthorhombic, rhombohedral, tetragonal, hexagonal, cubic.

The fundamental subsequent problem studied by BRAVAIS (and before also by FRANKENHEIM and CAUCHY) was then:
To find which 1-lattices are left invariant by the 32 crystallographic point groups (or indeed, by the 7 maximal ones). Also, for any crystal system, to classify all distinct simple lattices whose symmetry group belongs to that system.

Here, the meaning of distinct is not so obvious – Frankenheim and earlier authors had been unclear, and made ‘mistakes’. Bravais strives for clarity, and says:
“Deux Assemblages de la même classe appartiennent à des modes distincts de symétrie, lorsqu’en faisant varier d’une manière continue les espacements des Sommets de l’un des Assemblages, sans qu’il perde un seul instant ses axes de symétrie, on ne peut, malgré cela, le rendre que partiellement superposable avec l’autre Assemblage.”

That is: two lattices are of the same type when one is deformable onto the other without loss of symmetry elements (i.e., without lowering the crystal system) all along the deformation.

With this notion BRAVAIS (1850) finds the classical 14 lattice types that bear his name, representatives of which are presented in almost all references on crystallography.

REMARK 1: several lattice types belong in general to same crystal system. For instance, body-centered, face-centered and primitive cubic lattices are all in the cubic system. But the distinction of lattice type is very important, also physically: the bcc-fcc transformation in iron is perhaps the most important one in metallurgy.

REMARK 2: Bravais identified as distinct the primitive and the base-centered orthorhombic lattices. However, unrelated to this classification problem, ERICKSEN (1979) noticed that they can be deformed one onto the other without lowering the crystal system. The deformation of a suitable lattice basis is sketched below; the third lattice vector is orthogonal to the paper and can be regarded as constant along the deformation.

So, it is not clear whether the deformation criterion is the ‘correct’ one.

3. ‘ARITHMETIC’ SYMMETRY OF SIMPLE LATTICES

At the turn of the century, workers had started a parallel line of thinking, leading to a different criterion, for long thought to be equivalent to the original one by Bravais.

Recall: the problem is to define what it means for two lattices to be ‘distinct’. To do this we look at the basic relation (3) differently. Before we put the attention on the left-hand side, thus obtaining the crystallographic point groups. Now we rather look at the right-hand side, and introduce the lattice group \( L(e_a) \) of a lattice \( L(e_a) \): it is the group of integral matrices representing the lattice symmetries \( e_a \):

\[
L(e_a) = \{ m \in GL(3, \mathbb{Z}) : m^b e_b = Q e_a, Q \in P(e_a) \}. 
\]

Now, consider two simple lattices \( L = L(e_a) \) and \( \bar{L} = L(\bar{e}_a) \) and their lattice groups.

DEFINITION: \( L \) and \( \bar{L} \) are of the same Bravais type iff for suitable choices of their bases \( e_a \) and \( \bar{e}_a \) they have the same lattice group – that is, the same integral matrices representing their symmetries. Equivalently: \( L \) and \( \bar{L} \) are of the same Bravais type iff their lattice groups are ‘arithmetically’ equivalent, that is, conjugate in \( GL(3, \mathbb{Z}) \) – not in \( O(3) \).

In 2-d the analogue holds with \( GL(2, \mathbb{Z}) \).

With this definition one analyzes the lattice types by studying the conjugacy classes of lattice groups in \( GL(3, \mathbb{Z}) \) and \( GL(2, \mathbb{Z}) \). This led to the following definitive
THEOREM (BURKHARDT, circa 1930): There are 5 types of lattices in 2 dimensions, and 14 types in 3 dimensions. (So, BRAVAIS had the right answer anyway.)

The 5 two-dimensional lattice types

Since by (3) any matrix representation of $P(e_a)$ is linearly conjugate to $L(e_a)$, we see why there are 14 lattice types but only 7 crystal systems: it is easier to conjugate two matrices within $O(3)$ (or linearly) than within $GL(3, \mathbb{Z})$, since in the first case there are more possible conjugants. As a counterpart, the arithmetic symmetry, through the lattice groups, discriminates changes in symmetry, and possible transitions, better than geometric symmetry does through the crystal systems.

The arithmetic symmetry of lattices is closely related to the problem of the arithmetic equivalence of quadratic forms, studied by LAGRANGE, DIRICHLET, JORDAN, SOHNCKE, NIGGLI. To see how this relates to continuous deformations of lattices, we first stress that, up to orthogonal transformations, a simple lattice is characterized not by the lattice basis $e_a$ but rather by the corresponding symmetric positive-definite matrix (‘lattice metric’) $C_{ab} = e_a \cdot e_b$. Next, we exemplify in the 2-D case: the change of basis (1) comports an action of $GL(2, \mathbb{Z})$ on the 3-dimensional space $\mathbb{C}C^+_2$ of lattice metrics:

$$C \mapsto m^t C m, \quad C = C^t > 0, \quad m \in GL(2, \mathbb{Z}).$$

To study deformable lattices one analyzes the subspaces of $\mathbb{C}C^+_2$ left pointwise invariant by some (finite) subgroup of $GL(2, \mathbb{Z})$. Since changes in symmetry are unaffected by dilations, it is convenient to work with the following projective representation of $\mathbb{C}C^+_2$:

For instance, this picture shows that lowering the symmetry of a hexagonal net to rectangular in a continuous fashion, one necessarily obtains a centered rectangular lattice type.
In the same way $GL(3, \mathbb{Z})$ acts on $\mathcal{C}^+(\mathbb{Q}_3)$. For us, the 3-d framework is much more interesting; however the details of this action are known only locally, in a neighborhood of any point of $\mathcal{C}^+(\mathbb{Q}_3)$.

4. OUTLINE OF AN EXTENSION TO n-LATTICES (alloys, hcp metals, ...)

An n-lattice $\mathcal{M}$ in 3-d affine space can be defined as follows: (origin $O$, $p_0 = 0$)

$$\mathcal{M}(e_a, p_1, \ldots, p_{n-1}) = \bigcup_{i=0}^{n-1} \{O + \mathcal{L}(e_a) + p_i\}$$

The multilattice descriptors $(e_a, p_i) = e_a$ must satisfy the conditions $e_1 \cdot e_2 \times e_3 \neq 0$, $p_i \neq l_i^ae_a$, and $p_i \neq p_j + l_j^ae_a$, expressing three-dimensionality and non-overlap of the constituent simple lattices.

The geometric symmetry of n-lattices is classically studied through the space groups, i.e. the groups of affine isometries leaving some multilattice invariant. The classification of space groups was obtained at the turn of the century (JORDAN, SCHÖNFLIES, FEDOROV, FROBENIUS): There exist 217 affine conjugacy classes of space groups in three dimensions. Equivalence of the classifications by group isomorphism or affine conjugacy constitutes a famous theorem by BIEBERBACH solving the second part of HILBERT’s 18th problem.

The use of space groups in the analysis of multilattice symmetry has the same drawback as the use of crystal systems for 1-lattices: it is too coarse. Indeed, many distinct ‘types’ of multilattices may be compatible with the same space group. To mineralogists and metallurgists this is known; yet in crystallography there is no definition making the notion of ‘distinct multilattice types’ precise. Only empirical catalogues of structures are available. The Strukturberichte, very widely used but lacking a theoretical basis, are perhaps the most famous compilation.

We claim that the study of the arithmetic symmetry of multilattices gives the needed group-theoretical framework. It originated from the need of keeping track in a detailed way of the symmetry changes in deformable multilattices (phase transitions, etc.), and for describing correctly the invariance of their constitutive equations. The arithmetic symmetry of multilattices is introduced by mimicking the procedure for 1-lattices.

**First step:** replace the descriptors $e_a$ –see above– by the $O(3)$-invariant multilattice metric $K = (K_{a\tau})$, $K_{a\tau} = K_{\tau a} = e_a \cdot e_\tau$, $a, \tau = 1, \ldots, n-1$.

The manifold of multilattice metrics $\mathcal{Q}^n_{n+2}$ is a submanifold of the vector space $\mathcal{Q}_{n+2}$ of all symmetric matrices: $\mathcal{Q}^n_{n+2}$ is a ‘state space’ for n-lattices analogous to $\mathcal{C}^+(\mathbb{Q}_3)$ for 1-lattices.

**Second step:** identify the ‘global symmetry group’ of n-lattices, which must act on $\mathcal{Q}^n_{n+2}$ (recall the action of $GL(3, \mathbb{Z})$ on $\mathcal{C}^+(\mathbb{Q}_3)$). This is a consequence of the following
PROPOSITION: Let $\mathcal{M}(\varepsilon_\sigma)$ be a (monatomic) n-lattice. Then $\tilde{\varepsilon}_\sigma$ are new descriptors for $\mathcal{M}$ up to a translation (that is, $\mathcal{M}(\tilde{\varepsilon}_\sigma) = \mathcal{M}(\varepsilon_\sigma) + t$) if and only if there exists a suitable matrix $\mu$ such that $\tilde{\varepsilon}_\sigma = \mu^T \varepsilon_\sigma$; the matrix $\mu$ has the following form, for $a, b = 1, 2, 3, i, j = 1, \ldots, n - 1$, $(m_a^b, l_i^b) \in GL(3, \mathbb{Z})$, $l_i^b \in \mathbb{Z}$, and $\alpha = (\alpha_i^j)$ belonging to the finite non-commutative group of matrices generated by the permutation matrices of the set $\{1, \ldots, n-1\}$ and by the $n-1$ by $n-1$ matrices of the form $\tilde{\alpha}$ below, which are obtained from the identity by replacing one of its rows by a row of $-1$s:

$$
(\mu^T_\sigma) = \begin{pmatrix}
m_a^b & l_1^b & \cdots & l_{n-1}^b \\
0 & 0 & 0 & 0 \\
\vdots & \alpha_i^j & \ddots & \vdots \\
0 & 0 & 0 & 0
\end{pmatrix}, \quad \tilde{\alpha} = \begin{pmatrix}
1 & 0 & \cdots & 0 & 0 \\
1 & 0 & \cdots & 0 & 0 \\
\vdots & \ddots & \ddots & \vdots & \vdots \\
-1 & -1 & \cdots & -1 & -1 \\
0 & 0 & \cdots & 1 & 0 \\
0 & 0 & \cdots & 0 & 1
\end{pmatrix}.
$$

The matrix $\mu$ determines uniquely the new descriptors $\tilde{\varepsilon}_\sigma$, and vice versa.

The group of the above matrices $\mu$ is denoted by $\Gamma_{n+2}$, and it acts on a natural way on the space of multilattice metrics:

$$
K \mapsto \mu' K \mu.
$$

The study of the conjugacy classes of the subgroups of $\Gamma_{n+2}$ formalizes the notion of distinct (arithmetic) n-lattice types. The study of the action of $\Gamma_{n+2}$ on the state space $Q_{n+2}^m$ gives information on the kinematics of deformable n-lattices.

These studies are only at the beginning; contributors are ERICKSEN, ADELEKE, FADDA & ZANZOTTO, the latter having classified the monatomic 2-lattices in 2D and 3D, with interesting improvements over the Strukturbericht.

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FURTHER READING

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