# Bravais lattices associated with incommensurate crystal phases

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The symmetry of crystals with a periodic modulation can be described by means of superspace groups [1]. These are space groups of dimensionality higher than that of the crystal considered. Indeed in order to take into account both the periodicities of a basic structure and of the modulation, the n-dim. space $V_E$ spanned by the lattice $\Lambda$ of the basic structure (called external, or position space because it is the space in which the atoms are located) is extended by a d-dim. space $V_I$ (called internal space) spanned by the lattice D expressing the periodicity of the modulation. $V_S = V_E + V_I$ is then a (n+d) euclidean space called superspace. The density function $\rho$ describing the crystal appears then as the $V_E$-section of a scalar function $\rho$ (defined in $V_S$ and invariant with respect to a superspace group [2].

A (n,d)-dim. superspace group G is a subgroup of the euclidean group E(n+d) such that

(D1) $G \cap T(n+d) = \Sigma \simeq Z^{n+d}$, and $\Sigma$ generates $V_S$

(D2) $G \cap T(d) = D \simeq Z^d$ and D generates $V_I$

(D3) D is normal in G.

The first condition implies that G is a (n+d) dim space group. The second condition says that the new admitted translations (the internal ones) form a d-dim lattice D. The third condition implies that $G \subset E(n) \times E(d)$.

Due to the additional structure of the space group G, its subgroup of lattice translations $\Sigma$ and its point group K also have additional properties. In particular one has:

$$\Sigma \cap V_I = D \quad \text{and} \quad \pi_E \Sigma = \Lambda \tag{1}$$

where $\pi_E$ is the orthogonal projection of $V_S$ on $V_E$. Therefore we write $\Sigma = \Sigma(\Lambda,D)$. Considering the metric tensors $g_\Sigma$, $g_\Lambda$ and $g_D$ of lattice bases of $\Sigma$, $\Lambda$ and D respectively, their mutual relation (in matrix form) is:

$$g_\Sigma = \begin{pmatrix} g_\Lambda + \tilde{\sigma}\, g_D\, \sigma & -\tilde{\sigma} g_D \\ -g_D\, \sigma & g_D \end{pmatrix} \tag{2}$$

where $\sigma$ is a dxn real matrix and $\tilde{\sigma}$ its transposed.

The point group K being a subgroup of $O(n) \times O(d)$ its elements can be written in the form $R = (R_E, R_I)$. The components $R_E$ generate a n-dim. point

group $K_E \subset O(n)$ and the components $R_I$ a d-dim. point group $K_I \subset O(d)$.
For expressing this additional property we write $K = K(K_E, K_I)$, and we call it a (n,d) dim. point group.
Its main properties are:

(3) $\quad K\Sigma = \Sigma$ , $K_E \Lambda = \Lambda$ and $K_I D = D$

The choice of a so called standard lattice basis of $\Sigma$ characterized by the fact that its last d basis vectors lie in $V_I$ defines an integral faithful representation $\Gamma$ of K which has the (n,d) reduced form

(4) $$\Gamma(R) = \begin{pmatrix} \Gamma_E(R) & 0 \\ \Gamma_M(R) & \Gamma_I(R) \end{pmatrix} \in G\ell(n,d,Z)$$

with $\Gamma_E(R) \in G\ell(n,Z)$ and $\Gamma_I(R) \in G\ell(d,Z)$, whereas $G\ell(n,d,Z)$ is the subgroup of $G\ell(n+d,Z)$ of these (n,d) reduced elements. One has

(5) $\quad \tilde{\Gamma}_E(R)\, g_\Lambda\, \Gamma_E(R) = g_\Lambda$ , $\tilde{\Gamma}_I(R)\, g_D\, \Gamma_I(R) = g_D$ and

(6) $\quad \Gamma_M(R) = \sigma\Gamma_E(R) - \Gamma_I(R)\sigma$

Equivalence between (n,d) dim. superspace group G, G' implies the existence of an isomorphism $\chi: G \longrightarrow G'$ which maps the (unique) subgroup of internal translations D of G on the corresponding one D' of G'. Such an equivalence relation implies an (extended) arithmetic equivalence between point group representations $\Gamma(K)$ and $\Gamma'(K')$ as above:

(7) $\quad \Gamma(K) \simeq \Gamma'(K') \leftrightarrow \Gamma'(K') = S^{-1}\Gamma(K)\, S$ for a $S \in G\ell(n,d,Z)$.

Defining now the holohedry H of the lattice translation group $\Sigma(\Lambda,D)$ of G by:

(8) $\quad H = \{R \in O(n) \times O(d) \mid R\Sigma(\Lambda,D) = \Sigma(\Lambda,D)\}$

one shows,in the same way as for usual space group that lattice translations groups $\Sigma$ and $\Sigma'$ of equivalent superspace groups form an equivalence class among (n,d) dim. lattice translation groups also called Bravais class. Bravais equivalence is defined by:

(9) $\quad \Sigma \overset{B}{\sim} \Sigma' \leftrightarrow \Gamma(H) \overset{a}{\sim} \Gamma'(H')$

where H is the holohedry of $\Sigma(\Lambda,D)$ and H' that of $\Sigma'(\Lambda',D')$. Until now, no hypothesis were made on incommensurability. Incommensurability of the modulation implies at least a irrational matrix element $\sigma_{jk}$. We then say that the j-colum and k-row of $\sigma$ are incommensurable. In the incommensurate case the euclidean symmetry of the crystal density function $\rho$ is not a n-dim. space group. The modulated crystal structures considered in previous publications suppose that all rows of $\sigma$ are incommensurable, and that this property is invariant with respect to integral linear combinations of row vectors: We now call this the type I case. For this case and dimensions $n = 1,2,3$, and $d \leqslant n$ Bravais lattices have been derived. The original idea of listing all of them here could not be realized because of editorial limitations. For such a list and details on the method of derivation we refer to forthcoming publications.

A representative lattice $\Sigma$ from a Bravais class can be given either by its metric tensor or by its holohedry K with respect to a standard basis. The metric tensor $g_\Sigma$ in turn is determined by $g_\Lambda$, $g_D$ and $\sigma$ according to eq. (2). The elements $\Gamma_E(R)$ for $R \in K$ form an arithmetic point group in n dimensions. Hence it can be given in the usual crystallographic notation. For a type I lattice there is an element $\Gamma_I(R)$ for each element $\Gamma_E(R)$. These elements $\Gamma_I(R)$ form an arithmetic point group in d dimensions. Finally the arithmetic holohedry $\Gamma(K)$ is equivalent over the rationals to the fully reduced $\{(\Gamma_E(R) \oplus \Gamma_I(R)), R \in K\}$. Hence the lattice $\Sigma$ can be considered as a centering of a lattice with fully reduced holohedry. These points suggest a notation for the Bravais classes.

As an example we take Bravais class $C^{P\bar{3}m}_{\cdot\bar{1}1}$. The elements $\Gamma_E(R)$ form a point group $P\bar{3}m$ with generators

$$\bar{3} = \begin{pmatrix} 1 & 1 & 0 \\ -1 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad m = \begin{pmatrix} 1 & 1 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The holohedry $\Gamma(K)$ is generated by

$$\frac{\bar{3}}{\bar{1}} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 1 & 0 & -1 \end{pmatrix}, \quad \frac{m}{1} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$$

The lattice is centering of a lattice $P^{P6/mmm}_{\cdot 1\bar{1}1}$ with holohedry generated by

$$\frac{\bar{3}}{\bar{1}} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix}, \quad \frac{m}{1} = \begin{pmatrix} 1 & 1 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \quad \frac{6}{1} = \begin{pmatrix} 0 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

The fact that it is a centering is denoted by the letter C in front. The corresponding metric tensor follows from eq. (2) using

$$g_\Lambda = \begin{pmatrix} a^2 & \frac{1}{2}a^2 & 0 \\ \frac{1}{2}a^2 & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}, \quad g_D = d^2, \quad \sigma = \left( \frac{1}{3} \; \frac{2}{3} \; \gamma \right)$$

## References

1) A. Janner and T. Janssen, Phys.Rev. B15 (1977) 643.

2) P.M. de Wolff, Acta Cryst. A30 (1974) 777.