teaching and education

The Bravais polar lattice as a didactic tool for diffraction beginners

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When undergraduate students discover crystallography for the first time, they are usually already familiar with the phenomenon of diffraction as the 'bending' of waves around small obstacles. The special (periodic) nature of crystals acting as 'diffraction gratings' that produce interference of diffracted waves is typically rationalized in terms of the reciprocal lattice of the crystal. The concept of the reciprocal lattice, however, remains somewhat abstract for beginners, until they perform a diffraction experiment. It can be made more easily understandable through an intermediate step, namely its ancestor, the Bravais polar lattice. By means of a short historical trip through pre-X-ray crystallography, a generalized introduction to the notion of the dual lattice is given, of which the reciprocal lattice is the most common but by no means the only example, and it is shown how the use of the Bravais polar lattice can ease the introduction of the reciprocal lattice.

1. Some history: the idea behind the polar lattice

The atomic positions in a crystalline solid are usually described by fractional coordinates inside the unit cell, and the periodicity of the atomic distribution is expressed through the Bravais lattice. [The derivation of the independent types of lattices in three-dimensional space was first obtained by Frankenheim (1842), who obtained a number of 15. It was Bravais (1850; English translation by Shaler, 1949) who found the correct number of 14, and the three-dimensional lattices are now universally known as Bravais lattices.] The points of the Bravais lattice are those points to which a fixed corner of the unit cell can be moved by a translational symmetry of the crystal. The Bravais lattices express the periodicity in the space that physically contains the crystals and where we observe them. This space is usually called point space in crystallography, or, in particular when decorated with atoms, direct space. The concept of a crystal lattice in point space is very well established and normally its introduction in undergraduate courses does not present difficulties.

Until the beginning of the 20th century, crystals were studied morphologically, optically, and by physical and chemical tests, but there were no direct means to determine their atomic structure. With the discovery of X-rays, and the pioneer experiments on their diffraction by crystals (Friedrich et al., 1912), scientists working on condensed matter had a new world accessible to them. To interpret the diffraction pattern produced when a crystal is subject to an X-ray beam, the

concept of the reciprocal lattice was introduced (Ewald, 1913, 1921), and the lattice in point space was then renamed the direct lattice, the two being naturally dual to each other.

Actually, Ewald did not conjure the concept of the reciprocal lattice out of a magic hat: well before Ewald, Gibbs (1881; reprinted by Yale University, 1947; http://www.archive.org/details/117714283) had introduced a *reciprocal system of vectors*, for which $\mathbf{a}_i \cdot \mathbf{a}_j{}^* = \delta_{ij}$, i.e. precisely the same mathematical definition that is often used to introduce the reciprocal lattice. However, well before Gibbs, Bravais (1850) had introduced what is the true ancestor of the reciprocal lattice: a lattice dual to the direct lattice, which is nevertheless not reciprocal to it because its parameters are measured in ångströms, and not in ångströms^{-1}. It is called the polar lattice and played an important role in the study of crystal morphology.

As is well known, the law of the constancy of interfacial angles (Stenon's law) states that interfacial angles between corresponding faces are constant. The relative development (size) of a face, and even its presence, depends on the growth conditions of the crystal and represents an accessory feature. The most evident consequence is that the habitus – the external shape of a crystal – may not reveal much about its symmetry. This is a common trap for students, because the eye is caught by the relative *sizes* of the faces, whereas it is their *orientation* that reflects the symmetry of the crystal. When studying wooden crystal models, for example, one must always be careful to stress that those models (usually) represent an

idealized crystal, and that the relative sizes of the faces may be substantially different, although their relative orientation remains unchanged. In order to eliminate the effect of the accessory character of the crystal and to retain the essential features, the study of crystal morphology is performed by taking, from the centre of the crystal, the directions normal to each face, extended to intersect a sphere circumscribed around the crystal. These intersections, called spherical poles, are either projected onto a plane passing through the centre of the sphere, resulting in the stereographic projection, or are extended to reach a plane tangential to the sphere, giving the gnomonic projection (see, for example, Barker, 1922; Terpstra & Codd, 1961). The difference between these projections is the position of the point of sight (at the centre of the sphere or on the surface of it, respectively), while the common feature is precisely the elimination of the accessory character of the crystal – the relative size of the faces. The angle between the normals of two dihedral faces is taken as the angle between the faces, although it is actually the supplement of it: this comes from the way these angles are actually measured, namely by finding the orientation of the crystal, mounted on an optical goniometer, corresponding to the directions producing a reflection of the light incident on the faces.

A crystal face is simply the last plane of a family (hkl). Although the number of families is infinite, clearly only a limited number of faces can develop in the crystal morphology: the development of a face is in fact related to the growth conditions and the density of atoms (Bravais–Donnay–Harker law; Donnay & Harker, 1937). When the construction of a set of normals is performed on all the families of planes (hkl) and not only on the faces developed in the crystal habitus, the set of poles obtained when the normals are extended to meet the sphere represents the families of planes. However, the metric part of the information, namely the interplanar distance $d_{(hkl)}$, is lost. This metrical information was added by Bravais (1850), who transformed the set of *directions* normal to the families (hkl) to a system of *vectors*, each vector having a norm directly related to $d_{(hkl)}$. The periodic repetition of these vectors builds up a lattice that is dual to the original (direct) lattice, because the same construction applied twice returns to the original lattice. Because the intersections of the normals to the families (hkl) with the sphere circumscribed around the crystal are called poles, Bravais' construction was called the polar lattice ('*réseau polaire*' in the French original).

2. Construction of the polar lattice

The volume of the three-dimensional unit cell based on the three basis vectors **a**, **b** and **c** is

$$V = \mathbf{a} \cdot \mathbf{b} \times \mathbf{c} = \mathbf{b} \cdot \mathbf{c} \times \mathbf{a} = \mathbf{c} \cdot \mathbf{a} \times \mathbf{b}$$
$$= |\mathbf{a}||\mathbf{b}||\mathbf{c}| \left(1 - \cos^2 \alpha - \cos^2 \beta - \cos^2 \gamma + 2 \cos \alpha \cos \beta \cos \gamma\right)^{1/2}$$
$$= [\det(\mathbf{G})]^{1/2}, \tag{1}$$

where **G** is the metric tensor containing the dot products of the basis vectors. The norm $|\mathbf{a} \times \mathbf{b}|$ is the surface of the two-

dimensional cell defined by the vectors **a** and **b**, which Bravais indicated as $S(001)$. It corresponds to a vector normal to (001), the norm of which is $|\mathbf{a}||\mathbf{b}| \sin \gamma$. The scalar product of **c** and a unit vector perpendicular to (001), *i.e.* $\mathbf{c} \cdot (\mathbf{a} \times \mathbf{b})/|\mathbf{a} \times \mathbf{b}|$, gives the perpendicular distance between two planes of the (001) family, *i.e.* $d_{(001)}$ (Fig. 1). The volume of the unit cell can therefore be expressed as $V = S(001)d_{(001)}$. This result is immediately generalized to any family (hkl) because all cells with the same multiplicity have the same volume. Therefore, the volume of the unit cell is $V = S(hkl)d_{(hkl)}$, provided that the multiplicity is kept unchanged when changing the family of planes.

Bravais took a coordinate system $O\mathbf{abc}$, defining a primitive unit cell of volume V, and drew from the origin O the normals to three conjugated planes of the lattice. On each of these normals he marked a series of equidistant points, $S(hkl)/V^{1/3}$ apart. The factor $S(hkl)$ makes the distance between these points proportional to the size of the two-dimensional cell of the (hkl) family of lattice planes. The cube root of V is a normalization factor corresponding to the mean distance between the nodes of a lattice, *i.e.* the side of a cube having the same volume as the primitive unit cell of the lattice. As will be demonstrated, this normalization is required to obtain a unit cell of the same volume as the unit cell of the original lattice. Bravais' construction produces a new axial setting, $O\mathbf{a}^{\mathrm{P}}\mathbf{b}^{\mathrm{P}}\mathbf{c}^{\mathrm{P}}$, the basis vectors of which have parameters $S(100)/V^{1/3}$, $S(010)/V^{1/3}$ and $S(001)/V^{1/3}$ (Fig. 2).

The lattice built on $O\mathbf{a}^{\mathrm{P}}\mathbf{b}^{\mathrm{P}}\mathbf{c}^{\mathrm{P}}$ is the polar lattice (indicated by the superscript p) and has, evidently, the same dimensions as the original lattice, namely ångströms. A row $[hkl]^{\mathrm{P}}$ of the polar lattice corresponds to each family (hkl) of the original lattice. The period of $[hkl]^{\mathrm{P}}$ is the norm of the vector from the origin to the first node along this row, *i.e.* by construction

$$|\mathbf{r}^{\mathrm{P}}| = \frac{S(hkl)}{V^{1/3}} = \frac{V/d_{(hkl)}}{V^{1/3}} = \frac{V^{2/3}}{d_{(hkl)}}. \tag{2}$$

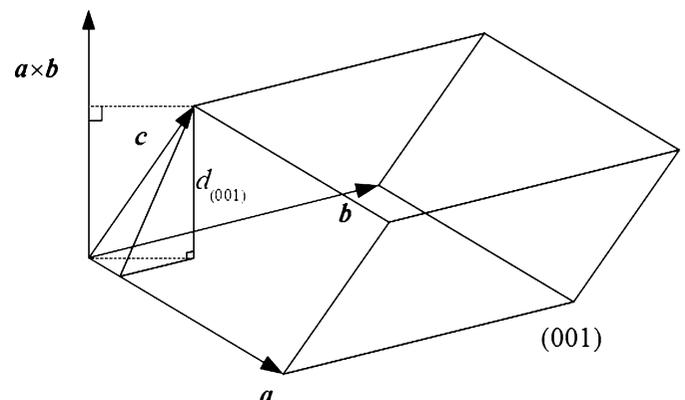In particular, the cell parameters of the polar lattice are

Figure 1
The interplanar distance of the (001) family.

$$\mathbf{a}^{\mathrm{p}} = \frac{S(100)}{V^{1/3}}\mathbf{u}_a = \frac{\mathbf{b} \times \mathbf{c}}{V^{1/3}},$$

$$\mathbf{b}^{\mathrm{p}} = \frac{S(010)}{V^{1/3}}\mathbf{u}_b = \frac{\mathbf{c} \times \mathbf{a}}{V^{1/3}}, \qquad (3)$$

$$\mathbf{c}^{\mathrm{p}} = \frac{S(001)}{V^{1/3}}\mathbf{u}_c = \frac{\mathbf{a} \times \mathbf{b}}{V^{1/3}},$$

where $\mathbf{u}_v$ is a unit vector in the direction of $\mathbf{v}^{\mathrm{p}}$.

Let $\mathbf{B}$ be the 3×3 matrix with $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ as its columns, and let $\mathbf{B}^{\mathrm{p}}$ be the matrix with $\mathbf{a}^{\mathrm{p}}$, $\mathbf{b}^{\mathrm{p}}$ and $\mathbf{c}^{\mathrm{p}}$ as its columns. By the definition of the basis of the polar lattice, we have

$$\mathbf{v}_i \cdot \mathbf{v}_j^{\mathrm{p}} = k\delta_{ij}, \quad k = V^{2/3}, \qquad (4)$$

from which one sees that $\mathbf{B}^{\mathrm{T}}\mathbf{B}^{\mathrm{p}} = V^{2/3}\mathbf{I}_3$, where $\mathbf{I}_3$ is the 3×3 identity matrix. This means that $\mathbf{B}^{\mathrm{p}} = V^{2/3}\mathbf{B}^{-\mathrm{T}}$ and $(\mathbf{B}^{\mathrm{p}})^{\mathrm{T}} = V^{2/3}\mathbf{B}^{-1}$.

For the metric tensors, this gives $\mathbf{G} = \mathbf{B}^{\mathrm{T}}\mathbf{B}$ and $\mathbf{G}^{\mathrm{p}} = (\mathbf{B}^{\mathrm{p}})^{\mathrm{T}}\mathbf{B}^{\mathrm{p}} = V^{2/3}\mathbf{B}^{-1}V^{2/3}\mathbf{B}^{-\mathrm{T}} = V^{4/3}\mathbf{G}^{-1}$. In particular, one has $\det(\mathbf{G}^{\mathrm{p}}) = (V^{4/3})^3/\det(\mathbf{G}) = V^4/V^2 = V^2$, and thus $V^{\mathrm{p}} = V$, *i.e.*

$$V^{\mathrm{p}} = \mathbf{a}^{\mathrm{p}} \cdot \mathbf{b}^{\mathrm{p}} \times \mathbf{c}^{\mathrm{p}} = \frac{\mathbf{b} \times \mathbf{c}}{V} \cdot \frac{\mathbf{c} \times \mathbf{a}}{V} \times \frac{\mathbf{a} \times \mathbf{b}}{V} = V. \qquad (5)$$

Bravais' normalization factor for the period along the lattice row $[hkl]^{\mathrm{p}}$ is thus chosen such that the unit cell of the polar lattice has the same size as that of the original lattice.

The result that taking the polar lattice of the polar lattice yields the direct lattice can be derived algebraically from the fact that $\mathbf{B}^{\mathrm{p}} = V^{2/3}\mathbf{B}^{-\mathrm{T}}$, since this implies $(\mathbf{B}^{\mathrm{p}})^{\mathrm{p}} = (V^{\mathrm{p}})^{2/3}(\mathbf{B}^{\mathrm{p}})^{-\mathrm{T}} = V^{2/3}(V^{2/3}\mathbf{B}^{-\mathrm{T}})^{-\mathrm{T}} = V^{2/3}(V^{-2/3}\mathbf{B}) = \mathbf{B}$, but it also follows directly from the properties of the vectors. By definition, $\mathbf{b}^{\mathrm{p}}$ is perpendicular to $\mathbf{a}$ and $\mathbf{c}$, and $\mathbf{c}^{\mathrm{p}}$ is perpendicular to $\mathbf{a}$ and $\mathbf{b}$, hence $\mathbf{a}$ is perpendicular to $\mathbf{b}^{\mathrm{p}}$ and $\mathbf{c}^{\mathrm{p}}$. Since also $(\mathbf{a}^{\mathrm{p}})^{\mathrm{p}}$ is perpendicular to $\mathbf{b}^{\mathrm{p}}$ and $\mathbf{c}^{\mathrm{p}}$, $\mathbf{a}$ and $(\mathbf{a}^{\mathrm{p}})^{\mathrm{p}}$ lie on the same line. Finally, since $\mathbf{a} \cdot \mathbf{a}^{\mathrm{p}} = \mathbf{a}^{\mathrm{p}} \cdot (\mathbf{a}^{\mathrm{p}})^{\mathrm{p}} = V^{2/3}$, $\mathbf{a}$ and $(\mathbf{a}^{\mathrm{p}})^{\mathrm{p}}$ actually have to be equal.

Determining the cell parameters is now straightforward. The norms of the basis vectors are

Figure 2
Definition of the basis vectors of the polar lattice.

$$a^{\mathrm{p}} = bc \sin\alpha/V^{1/3},$$

$$b^{\mathrm{p}} = ac \sin\beta/V^{1/3},$$

$$c^{\mathrm{p}} = ab \sin\gamma/V^{1/3},$$

$$a = b^{\mathrm{p}}c^{\mathrm{p}} \sin\alpha^{\mathrm{p}}/V^{1/3}, \qquad (6)$$

$$b = a^{\mathrm{p}}c^{\mathrm{p}} \sin\beta^{\mathrm{p}}/V^{1/3},$$

$$c = a^{\mathrm{p}}b^{\mathrm{p}} \sin\gamma^{\mathrm{p}}/V^{1/3},$$

taking $V^{\mathrm{p}} = V$. The interaxial angles are the supplement of the dihedral angles between corresponding planes,

$$\alpha^{\mathrm{p}} = \pi - (010)^{\wedge}(001),$$

$$\beta^{\mathrm{p}} = \pi - (100)^{\wedge}(001), \qquad (7)$$

$$\gamma^{\mathrm{p}} = \pi - (101)^{\wedge}(010),$$

and from equation (3) one obtains immediately

$$\sin\alpha^{\mathrm{p}} = \frac{aV^{1/3}}{b^{\mathrm{p}}c^{\mathrm{p}}} = \frac{aV^{1/3}}{\frac{ac\sin\beta}{V^{1/3}}\frac{ab\sin\gamma}{V^{1/3}}} = \frac{V}{abc\sin\beta\sin\gamma},$$

$$\sin\beta^{\mathrm{p}} = \frac{bV^{1/3}}{a^{\mathrm{p}}c^{\mathrm{p}}} = \frac{bV^{1/3}}{\frac{bc\sin\alpha}{V^{1/3}}\frac{ab\sin\gamma}{V^{1/3}}} = \frac{V}{abc\sin\alpha\sin\gamma}, \qquad (8)$$

$$\sin\gamma^{\mathrm{p}} = \frac{cV^{1/3}}{a^{\mathrm{p}}b^{\mathrm{p}}} = \frac{cV^{1/3}}{\frac{bc\sin\alpha}{V^{1/3}}\frac{ac\sin\beta}{V^{1/3}}} = \frac{V}{abc\sin\alpha\sin\beta}.$$

The polar lattice turns out to be of the same type as the original lattice, with the exception of the F and I types, which are interchanged. Therefore, we find all the main features of the later reciprocal lattice but expressed in the same metric as the direct lattice. The polar lattice has the merit of being easily understandable by any student who has handled a couple of wooden models and has realized that the orientation of the faces, not their size, is the external character reflecting the true symmetry of the crystal. The dihedral angle (actually, the supplement of it, as we have seen) is easily computed as the angle φ between two vectors of the polar lattice,

$$\mathbf{r}_{hkl}^{\mathrm{p}} \cdot \mathbf{r}_{h'k'l'}^{\mathrm{p}'} = |\mathbf{r}_{hkl}^{\mathrm{p}}||\mathbf{r}_{h'k'l'}^{\mathrm{p}'}|\cos\varphi,$$

$$\cos\varphi = \mathbf{r}_{hkl}^{\mathrm{p}} \cdot \mathbf{r}_{h'k'l'}^{\mathrm{p}'}/|\mathbf{r}_{hkl}^{\mathrm{p}}||\mathbf{r}_{h'k'l'}^{\mathrm{p}'}|$$

$$= \frac{\langle\mathbf{hkl}|\mathbf{G}^{\mathrm{p}}|\mathbf{h'k'l'}\rangle}{(\langle\mathbf{hkl}|\mathbf{G}^{\mathrm{p}}|\mathbf{hkl}\rangle)^{1/2}(\langle\mathbf{h'k'l'}|\mathbf{G}^{\mathrm{p}}|\mathbf{h'k'l'}\rangle)^{1/2}}, \qquad (9)$$

where the *bra* $\langle\mathbf{hkl}|$ simply denotes the row vector (h,k,l) and the *ket* $|\mathbf{hkl}\rangle$ the column vector $(h,k,l)^{\mathrm{T}}$. The *bra* and *ket* (together forming a *bracket*) thus provide a convenient notation for the dot product calculation $\mathbf{v}^{\mathrm{T}} \cdot \mathbf{G} \cdot \mathbf{w}$ involving the metric tensor $\mathbf{G}$.

3. From the polar lattice to the reciprocal lattice

The discovery of the wave nature of the X-rays through their diffraction by a crystal (Friedrich *et al.*, 1912) led Ewald (1913, 1921) to introduce the notion of the reciprocal lattice, which rapidly replaced the polar lattice to the extent that the latter was almost completely forgotten, with the exception of a few citations in rare texts like Terpstra & Codd (1961), Brasseur (1967) (where it was, however, erroneously mentioned simply as a synonym of the reciprocal lattice) and Rigault (1999),
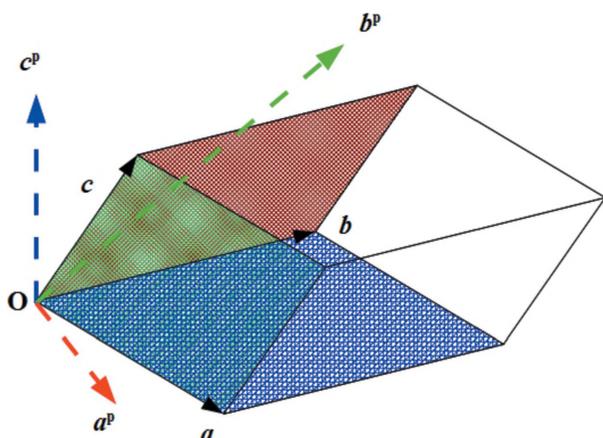
while it is not even mentioned in Volume B of *International Tables for Crystallography* (2008). Nowadays, it is common to introduce the reciprocal lattice in a rather axiomatic way, by imposing $k = 1$ in the analogue of equation (4) when $\mathbf{v}^P$ is replaced by $\mathbf{v}^*$ (see *e.g.* Giacovazzo *et al.*, 2002). Actually, the reciprocal lattice is more easily understood through a more physical introduction. The amplitude of a diffracted wave is proportional to the Fourier transform of the electron density of the scattering body, but the scaling properties of the Fourier transform lead to a metric of the space that is reciprocal to the metric of the direct space. By repeating the construction of the polar lattice but taking the period along the row $[hkl]^*$ as $1/d_{(hkl)}$ instead of $V^{2/3}/d_{(hkl)} = S(hkl)/V^{1/3}$ (thus obtaining vectors measured in Å^{-1} instead of Å), all the well known properties of the reciprocal lattice are immediately obtained, in particular

$$|\mathbf{r}^*| = 1/d_{(hkl)}, \tag{10}$$

$$\mathbf{a}^* = \frac{S(100)}{V}\mathbf{u}_a = \frac{\mathbf{b} \times \mathbf{c}}{V},$$
$$\mathbf{b}^* = \frac{S(010)}{V}\mathbf{u}_b = \frac{\mathbf{c} \times \mathbf{a}}{V}, \tag{11}$$
$$\mathbf{c}^* = \frac{S(001)}{V}\mathbf{u}_c = \frac{\mathbf{a} \times \mathbf{b}}{V},$$

$$\mathbf{v}_i \cdot \mathbf{v}_i^* = \mathbf{v}_i \cdot \frac{\mathbf{v}_j \times \mathbf{v}_k}{V} = 1, \tag{12}$$

$$V^* = \mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^* = \frac{\mathbf{b} \times \mathbf{c}}{V} \cdot \frac{\mathbf{c} \times \mathbf{a}}{V} \times \frac{\mathbf{a} \times \mathbf{b}}{V} = \frac{1}{V}. \tag{13}$$

Since $\mathbf{a}^* = \mathbf{a}^P/V^{2/3}$, $\mathbf{b}^* = \mathbf{b}^P/V^{2/3}$ and $\mathbf{c}^* = \mathbf{c}^P/V^{2/3}$, the interaxial angles for the reciprocal lattice are the same as those for the polar lattice, *i.e.* equation (8) remains unchanged.

Furthermore, for the metric tensor $\mathbf{G}^*$ we have $\mathbf{G}^* = V^{-4/3}\mathbf{G}^P = \mathbf{G}^{-1}$. From this, one sees that the dihedral angles for the reciprocal lattice are the same as for the polar lattice, since the scaling factor $V^{-4/3}$ cancels out:

$$\cos \varphi = \mathbf{r}^*_{hkl} \cdot \mathbf{r}^*_{h'k'l'}/|\mathbf{r}^*_{hkl}||\mathbf{r}^*_{h'k'l'}|$$
$$= \frac{\langle hkl|\mathbf{G}^*|h'k'l'\rangle}{(\langle hkl|\mathbf{G}^*|hkl\rangle)^{1/2}(\langle h'k'l'|\mathbf{G}^*|h'k'l'\rangle)^{1/2}}$$
$$= \mathbf{r}^P_{hkl} \cdot \mathbf{r}^{P'}_{h'k'l'}/|\mathbf{r}^P_{hkl}||\mathbf{r}^{P'}_{h'k'l'}|. \tag{14}$$

The introduction of the polar lattice is a natural consequence of Stenon's law and the introduction of the reciprocal metric is a natural consequence of Fraunhofer diffraction. Therefore, the polar lattice represents a useful didactic tool concretely related to the morphological analysis of crystals (or wooden models), through which the student becomes easily accustomed to working in a space that is dual to direct space. The transition to the reciprocal lattice is then just a small step further, justified by the passage to the reciprocal metric resulting from the Fourier nature of diffraction. It is realized by dividing the vectors of the polar lattice by $V^{2/3}$.

4. The polar lattice as a special case of the pseudo-reciprocal lattice

The polar and reciprocal lattices can actually both be seen as special cases of a generalized dual lattice, defined by taking a parametric value for k in equation (4) written for two dual bases $(\mathbf{v}_1, \ldots, \mathbf{v}_n)$ and $(\mathbf{w}_1, \ldots, \mathbf{w}_n)$. Grimmer (2003) introduced the term pseudo-reciprocal lattice for such a lattice, with the constraint, however, of having k of dimension length squared. If we remove this restriction, the pseudo-reciprocal lattice becomes the parent lattice of any lattice dual to the direct lattice. The reciprocal lattice is then clearly pseudo-reciprocal (with $k = 1$). Bravais' polar lattice is pseudo-reciprocal with $k = V^{2/3}$, complying also with Grimmer's original definition.

A particularly pleasing feature of the pseudo-reciprocal lattice is that it can actually be defined without recourse to the basis. We demonstrate this for the reciprocal lattice. Let L be a lattice with primitive lattice basis $(\mathbf{v}_1, \ldots, \mathbf{v}_n)$. Because the chosen basis is primitive, the vectors in L are all linear combinations of $\mathbf{v}_i$ ($i = 1, \ldots, n$) with integral coefficients. Let us then introduce a lattice $L^{\#}$ as the set of all vectors $\mathbf{r}$ in $\mathbb{R}^n$ having integral dot products with all the vectors in L, *i.e.*

$$L^{\#} := \{\mathbf{r} \in \mathbb{R}^n | \mathbf{v} \cdot \mathbf{r} \in \mathbb{Z} \text{ for all } \mathbf{v} \in L\}.$$

If we now consider the reciprocal lattice L^* with basis $(\mathbf{v}_1^*, \ldots, \mathbf{v}_n^*)$ as defined above, it is clear that $L^* \subseteq L^{\#}$, since $\mathbf{v}_i^*$ are contained in $L^{\#}$ (because all inner products $\mathbf{v}_i^* \cdot \mathbf{v}_j$ are integral). Conversely, any vector $\mathbf{r} \in L^{\#}$ can be expressed as a linear combination of the vectors $\mathbf{v}^* \in L^*$: $\mathbf{r} = \sum_{i=1}^n \lambda_i \mathbf{v}_i^*$ with $\lambda_i \in \mathbb{R}$. But $\mathbf{r} \cdot \mathbf{v}_i = \lambda_i$, and since $\mathbf{r} \in L^{\#}$ this gives $\lambda_i \in \mathbb{Z}$. Thus, $\mathbf{r}$ is an integral linear combination of the values of $\mathbf{v}_i^*$ and hence contained in L^*. For an arbitrary pseudo-reciprocal lattice with constant k, the above argument is easily modified and shows that the pseudo-reciprocal lattice consists of all vectors $\mathbf{r}$ in $\mathbb{R}^n$ having dot products in $k\mathbb{Z}$ with all vectors in L.

5. The antireciprocal lattice

Bravais' choice to take $V^{2/3}/d_{(hkl)}$ as the period along the rows of the dual lattice was quite evidently dictated by the desire that the length of the vector representing the (hkl) family of lattice planes should be proportional to the size of the two-dimensional cell in a plane of that family, and that the primitive unit cell of the new lattice should have the same volume as that of the direct lattice. A different natural choice is to take $d_{(hkl)}$ as the period along the lattice row perpendicular to the (hkl) family. Such an approach comes out quite naturally from a morphological analysis and is guided by the fundamental features of the (hkl) families of lattice planes, namely the orientation of the planes, as expressed by their normals, and the interplanar distance. For the vector $\mathbf{r}^a$ representing the (hkl) family one immediately obtains

$$|\mathbf{r}^a| = d_{(hkl)} = 1/|\mathbf{r}^*_{(hkl)}| = V^{2/3}/|\mathbf{r}^P|, \tag{15}$$

and this shows that some care must be taken with this approach. Since the vectors $\mathbf{r}^*_{hkl}$ are unrestricted in their

lengths, looking at all families (*hkl*) of lattice planes would produce vectors $\mathbf{r}^a$ of arbitrarily small length. Thus, running over all families (*hkl*), the corresponding vectors $\mathbf{r}^a$ do not form a lattice. In order to arrive at a lattice, we only construct the vectors $\mathbf{a}^a$, $\mathbf{b}^a$ and $\mathbf{c}^a$ for a primitive basis (**a**, **b**, **c**) and take ($\mathbf{a}^a$, $\mathbf{b}^a$, $\mathbf{c}^a$) as the primitive basis for a lattice that we call antireciprocal (indicated by the superscript a). Since the basis of the antireciprocal basis is defined exactly the same as that of the reciprocal lattice but with inverse parameters, we easily derive the analogous relations

$$\mathbf{a}^a = \frac{1}{|\mathbf{a}^*|}\mathbf{u}_a = \frac{\mathbf{a}^*}{|\mathbf{a}^*|^2} = \frac{V}{|\mathbf{b}\times\mathbf{c}|}\mathbf{u}_a = \frac{V^{2/3}}{|\mathbf{a}^p|}\mathbf{u}_a,$$

$$\mathbf{b}^a = \frac{1}{|\mathbf{b}^*|}\mathbf{u}_b = \frac{\mathbf{b}^*}{|\mathbf{b}^*|^2} = \frac{V}{|\mathbf{c}\times\mathbf{a}|}\mathbf{u}_b = \frac{V^{2/3}}{|\mathbf{b}^p|}\mathbf{u}_b, \qquad (16)$$

$$\mathbf{c}^a = \frac{1}{|\mathbf{c}^*|}\mathbf{u}_c = \frac{\mathbf{c}^*}{|\mathbf{c}^*|^2} = \frac{V}{|\mathbf{a}\times\mathbf{b}|}\mathbf{u}_c = \frac{V^{2/3}}{|\mathbf{c}^p|}\mathbf{u}_c,$$

$$\mathbf{v}_i \cdot \mathbf{v}_i^a = \mathbf{v}_i \cdot \frac{\mathbf{v}_i^*}{|\mathbf{v}_i^*|^2} = \frac{1}{|\mathbf{v}_i^*|^2} = d_i^2, \qquad (17)$$

$$V^a = \mathbf{a}^a \cdot \mathbf{b}^a \times \mathbf{c}^a = \frac{\mathbf{a}^* \cdot \mathbf{b}^* \times \mathbf{c}^*}{|\mathbf{a}^*|^2|\mathbf{b}^*|^2|\mathbf{c}^*|^2} = \frac{V^*}{|\mathbf{a}^*|^2|\mathbf{b}^*|^2|\mathbf{c}^*|^2}$$
$$= \frac{d_{100}^2 d_{010}^2 d_{001}^2}{V}. \qquad (18)$$

While taking $d_{(hkl)}$ as the period for the basis vectors of the antireciprocal lattice is very intuitive, the price to be paid for this is that the construction is basis-dependent. Equation (18) shows that the volume of the unit cell may change upon transition to a different basis of the direct lattice, since the interplanar distances may alter. Furthermore, the antireciprocal lattice is only pseudo-reciprocal if the interplanar distances $d_{(100)}$, $d_{(010)}$ and $d_{(001)}$ are all equal for the chosen basis (**a**, **b**, **c**).

5.1. Example

Let ($\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$) be a Cartesian (orthonormal) basis of $\mathbb{R}^3$ ($\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij}$) and L the standard lattice $\mathbb{Z}^3$. For this basis, the polar, reciprocal and antireciprocal lattices coincide. However, in crystallography a conventional basis is usually chosen to comply with the symmetry directions of the lattice. Let such a basis be (**a**, **b**, **c**), with $\mathbf{a} = (100)^T$, $\mathbf{b} = (110)^T$ and $\mathbf{c} = (001)^T$ with respect to ($\mathbf{e}_1$, $\mathbf{e}_2$, $\mathbf{e}_3$). Then $V = 1$ and, for the reciprocal basis ($\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$), one has $\mathbf{a}^* = (1\bar{1}0)^T$, $\mathbf{b}^* = (010)^T$ and $\mathbf{c}^* = (001)^T$, and $V^* = 1/V = 1$. For the antireciprocal basis ($\mathbf{a}^a$, $\mathbf{b}^a$, $\mathbf{c}^a$), however, one obtains $\mathbf{a}^a = \frac{1}{2}(1\bar{1}0)^T$, $\mathbf{b}^a = (010)^T$ and $\mathbf{c}^a = (001)^T$, giving volume $V^a = \frac{1}{2}$.

6. Deriving dual lattices from dual space

Underlying the concept of dual lattice is the much more abstract notion of dual space. Given a vector space **V**, its dual space **V*** is defined to be the space of linear functions (func-

tionals) from **V** to $\mathbb{R}$. Considering an element **v** of **V** as a column vector $(x_1, \ldots, x_n)^T$, a function φ is no more than a $1 \times n$ matrix $(u_1, \ldots, u_n)$ (*i.e.* a row vector), and the application of φ to **v** is simply $\varphi(\mathbf{v}) = u_1 x_1 + \cdots + u_n x_n$. However, this is just the usual dot product of the column vector $\mathbf{u} = (u_1, \ldots, u_n)^T$ with **v**. Thus, identifying row vectors with column vectors, **V*** is identified with **V** such that $\mathbf{u} \in \mathbf{V}$ gives rise to the function φ_u: $\mathbf{v} \mapsto \mathbf{u} \cdot \mathbf{v}$.

The vectors mapped to 0 by the function φ_u are precisely those vectors lying in the $(n-1)$-dimensional subspace (called a hyperplane) of **V** that is perpendicular to **u**, which represents the kernel of φ_u. *Vice versa*, for every $(n-1)$-dimensional subspace of **V** there is a function in **V*** (unique up to scalings) mapping this subspace to 0, namely φ_u such that **u** is perpendicular to the subspace. This makes it natural to define, for a given basis $(\mathbf{v}_1, \ldots, \mathbf{v}_n)$ of **V**, a basis $(\varphi_1, \ldots, \varphi_n)$ of **V*** such that $\varphi_i(\mathbf{v}_j) = \delta_{ij}$. With the identification of **V*** with **V**, the row vector φ_i read as a column vector is a vector $\mathbf{v}_i^*$, such that $\mathbf{v}_i^*$ is perpendicular to $\mathbf{v}_j$ for $j \neq i$ and $\mathbf{v}_i \cdot \mathbf{v}_i^* = 1$. The basis $(\mathbf{v}_1^*, \ldots, \mathbf{v}_n^*)$ is then called the dual basis of $(\mathbf{v}_1, \ldots, \mathbf{v}_n)$.

The different types of dual lattices share the property that they have a primitive basis of the form $(\lambda_1 \mathbf{v}_1^*, \lambda_2 \mathbf{v}_2^*, \ldots \lambda_n \mathbf{v}_n^*)$, *i.e.* such that the *i*th basis vector lies on the line perpendicular to all $\mathbf{v}_j$ with $j \neq i$.

For the special case of $\mathbf{V} = \mathbb{R}^3$, the vector product is a convenient means of finding the dual lattices, since for (**a**, **b**, **c**) the basis ($\mathbf{b} \times \mathbf{c}$, $\mathbf{c} \times \mathbf{a}$, $\mathbf{a} \times \mathbf{b}$) fulfils the required orthogonality conditions and the vectors only have to be scaled as desired.

We note that the two dual spaces occur naturally in crystallography. The point space E^n is an affine space with underlying vector space $\mathbf{V} = \mathbb{R}^n$, *i.e.* every point of E^n is obtained as the translation of a single (but arbitrary) point of E^n by all vectors of **V**. The dual space **V*** of **V** (identified with **V**) is the vector space in which the face normals and reciprocal lattice vectors reside.

7. Conclusions

The Bravais polar lattice is a natural intermediate between morphological and diffraction studies of crystals, both considering vectors that are normal to certain planes in direct space. The construction of the Bravais polar lattice is intuitive and facilitates a good understanding of the reciprocal lattice before any diffraction experiment is performed.

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