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A method of determining the coincidence site lattices for cubic crystals.

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A quick method is presented of determining the coincidence site lattice when the original lattice is primitive cubic.

In a paper by Grimmer, Bollmann & Warrington (1974), to which we shall refer as GBW, methods have been described for the determination of the coincidence site lattice when the original lattice is primitive cubic. The purpose of this note is to present a new method of determining this coincidence site lattice, a method which is quick and has a clear geometrical interpretation.

We shall closely follow the notation and conventions introduced in §§ 1·1 and 1·2 of GBW. The rotation $\mathbf{R}$ maps G_1^P, the primitive cubic lattice 1, into G_2^P. The translation vectors that belong simultaneously to G_1^P and G_2^P form the coincidence site lattice G_C^P. We consider rotations that, in an orthogonal coordinate system with axes parallel to the fourfold axes of G_1^P, are described by a matrix $\mathbf{R}$, the nine elements of which are rational numbers with a smallest common denominator N,

$$\mathbf{R}=\frac{1}{N}\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}.$$

N is odd and the a_{ij} are integers. We denote the column vectors of $\mathbf{R}$ by

$$\mathbf{e}_i=N^{-1}\{a_{1i}, a_{2i}, a_{3i}\}, \quad i=1,2,3 .$$

G_1^P consists of the vectors with integral components; G_2^P of the vectors $\mathbf{v}$ of the form

$$\mathbf{v}=n_1\mathbf{e}_1+n_2\mathbf{e}_2+n_3\mathbf{e}_3 ,$$

where the coefficients n_1, n_2, and n_3 are integers; the vectors of G_C^P have integral components and integral coefficients n_i. Denote the largest common divisor of the integers a_{1i}, a_{2i}, a_{3i} by α_i, $i=1,2,3$.

Theorem. There is a unique integer m satisfying $|m|<\frac{1}{2}N/\alpha_1$ such that $m\mathbf{e}_1+\alpha_1\mathbf{e}_2$ has integral coefficients. There is a unique pair of integers p, q satisfying $|p|<\frac{1}{2}N/\alpha_1$ and $|q|<\frac{1}{2}\alpha_1$ such that $p\mathbf{e}_1+q\mathbf{e}_2+\mathbf{e}_3$ has integral coefficients. The vectors

$$\mathbf{b}_1=N\,.\,\mathbf{e}_1/\alpha_1$$
$$\mathbf{b}_2=m\,.\,\mathbf{e}_1+\alpha_1\,.\,\mathbf{e}_2$$
$$\mathbf{b}_3=p\,.\,\mathbf{e}_1+q\,.\,\mathbf{e}_2+\mathbf{e}_3$$

form a basis for the coincidence site lattice G_C^P.

This theorem tells us that in order to find a basis for G_C^P we just have to check (by hand or computer) which of the N/α_1 possible values of m gives a vector $\mathbf{b}_2$ with integral components and which of the $\alpha_1\,.\,N/\alpha_1=N$ possible values of the pair p,q gives a vector $\mathbf{b}_3$ with integral components.

For the example discussed in §§ 1.5 and 2.2.1 of GBW we have

$$13\mathbf{e}_1=\{12,4,-3\}, \quad 13\mathbf{e}_2=\{-3,12,4\}, \quad 13\mathbf{e}_3=\{4,-3,12\}$$

and we obtain for Λ_C^P the basis

$$\mathbf{b}_1=\{12,4,-3\}, \quad \mathbf{b}_2=-3\mathbf{e}_1+\mathbf{e}_2=\{-3,0,1\}, \quad \mathbf{b}_3=4\mathbf{e}_1+\mathbf{e}_3=\{4,1,0\}.$$

For a given rotation $\mathbf{R}$, there is a close connexion between the coincidence site lattices of primitive cubic, b.c.c., and f.c.c. crystals and between the coincidence site lattices and the DSC lattices. For details we refer the reader to §§ 1.3 and 1.4 of GBW.

It remains to prove the theorem. $\mathbf{b}_1$ is the shortest vector in G_C^P that is parallel to $\mathbf{e}_1$. It follows from Lemma 2 in GBW that α_1 and α_2 have no common divisor. Therefore a vector of the form $m\mathbf{e}_1+n\mathbf{e}_2$, m and n integers, cannot have integral components unless n is a multiple of α_1. Let $\nu\,.\,\alpha_1$ denote the smallest positive value of n for which there is a vector of the form $m\mathbf{e}_1+n\mathbf{e}_2$ with integral components. Let us call 'lattice point' a point with position vector in G_2^P and 'coincidence site' a point with position vector in G_C^P. Since on two parallel straight lines that both contain coincidence sites these sites are the same distance apart, the ratio σ_π of lattice points to coincidence sites in the plane π spanned by $\mathbf{e}_1$ and $\mathbf{e}_2$ is $\nu\alpha_1\,.\,N/\alpha_1=\nu N$. It has been shown in the Appendix to GBW that $\Sigma=N$, Σ being the ratio of lattice points to coincidence sites in three-dimensional space. Consider two parallel planes that both contain coincidence sites. These sites form the same pattern in both planes, which shows that σ_π cannot be larger than Σ. We conclude that $\nu=1$ and that each lattice plane parallel to π contains coincidence sites. All the statements of the theorem on $\mathbf{b}_2$ and $\mathbf{b}_3$ follow immediately. We know now that $\mathbf{b}_1$, $\mathbf{b}_2$, and $\mathbf{b}_3$ belong to G_C^P; they form a basis for it because the parallelepiped with these vectors as edges has volume $V=N$,

$$V=\det\begin{pmatrix} N/\alpha_1 & 0 & 0 \\ m & \alpha_1 & 0 \\ p & q & 1 \end{pmatrix}=N.$$

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Reference

Grimmer, H., Bollmann, W. & Warrington, D. H. (1974). *Acta Cryst.* A**30**, 197–207.