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On the Geometry of Coincidence-Site Lattices

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A method involving inspection has been devised for deriving the angular values about an axis [*hkl*] in the cubic system which will lead to a coincidence-site lattice relationship. The idea of a generating function is used here in an extension of the procedures evolved by Frank for [100] and [111] rotations and by Dunn for [110] rotations.

Introduction

Rotational symmetry operations on a lattice bring it into complete self-coincidence. However, partial self-coincidence can occur for certain other rotations about an axis. Two crystal lattices related by such an angular rotation about an axis have certain common sites, located on a single lattice of larger cell dimensions. This larger lattice is called the coincidence-site lattice. The importance of such lattices in connexion with secondary recrystallization textures was first realized by Kronberg & Wilson (1949). Since then several investigators have used the concept of coincidence-site lattices in other contexts, for example, grain boundary migration in high purity materials (Aust & Rutter, 1959) and the structure of grain boundaries in diamond (Hornstra, 1960), in metals and alloys (Brandon, Ralph, Ranganathan & Wald, 1964) and in sphalerite (Holt, 1964). This continuing interest in the coincidence-site lattice model makes it worth while to consider a general approach to the generation of such lattices. The misorientation relationship between two crystals can be given as an axis–angle pair. It is the purpose of this article to derive the angular values about an axis [*hkl*] in the cubic system which will lead to a coincidence-site lattice relationship.

Previous work

Frank (1958) has indicated a procedure for obtaining coincidence-site lattices for rotations about [100] and [111]. His procedure for [100] is, briefly, as follows. A lattice point is chosen as the origin and a square cell is constructed on each line joining the origin to a visible point, where visibility is defined in the sense used by Hardy & Wright (1945) and indicates that there are no other points on the line between the given lattice point and the origin. It is seen that each such cell is a square cell of dimensions larger than those of the original unit cell and can be used to generate a coincidence-site lattice. The ratio of the area of the new square cell to that of the original lattice is x^2+y^2, where (x,y) are the cartesian coordinates of the lattice point which is joined to the origin. This ratio is also equal to the multiplicity, Σ, of the coincidence site lattice, which may be defined as the reciprocal of the density of common points. The procedure for [110] is more complicated as there are no squares. Dunn & Brandhorst (1958) and Dunn (1959) have worked out an extension of Frank's procedure. They essentially determine the area of a rectangle constructed on the line joining the origin to a visible point.

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Alternative approach

The work of Friedel (1926) permits the derivation of axis-angle pairs for coincidence by a different route. (Goux has pointed this out independently in a private communication). The rotation of 180° around [*hkl*] in the cubic system gives rise to a coincidence site lattice of $\Sigma=h^2+k^2+l^2$, if $h^2+k^2+l^2$ is odd or $(h^2+k^2+l^2)/2$, if $h^2+k^2+l^2$ is even. Also in the cubic system the relationship of [*hkl*]$-$180° can equally well be represented in twenty-three other ways. These twenty-four rotations which describe the same orientation relationship are just the combination of any particular original rotation with the 24 proper symmetry rotations associated with a cube having indistinguishable faces. The alternative relationships can be found by using analytical equations (Goux, 1961) or transformation matrices (Hornstra, 1960). This approach leaves the question of finding the possible Σ values for a given axis undecided.

Similar lattices

Coxeter (1948) has dealt with the problem of finding larger similar lattices without reference to lattice coincidence. He has termed them 'compound tessellations' and has given x^2+y^2 and x^2+xy+y^2 as generating functions for square and hexagonal lattices. The only restriction on x and y is that they should be non-negative integers. He has also shown that a square cell cannot be constructed on a hexagonal lattice and *vice versa.* This work provided the stimulus for discovering a generating function for coincidence-site lattices. It may be noted that Loeb (1964) has used the function x^2+xy+y^2 for finding structural possibilities for compounds. [These functions also have the entirely unsuspected property of giving the minimum number of colours necessary for maps on surfaces of varying complexity (*cf.* Coxeter, 1961)].

A generating function

Consider the two-dimensional rectangular lattice shown in Fig. 1. The axial ratio, R, of its unit cell is restricted to rational values. Each rotation of the lattice point $(x, -y)$ into (x,y) will give rise to a coincidence site lattice as the row on which $(x, -y)$ lies and the row perpendicular to it come into coincidence. The angle of the rotation is $2\tan^{-1}(y/x)R$. The area ratio, Σ, of the unit cell of the similar, large rectangular lattice to that of the original lattice is $x^2+R^2y^2$. The multiplicity, Σ_R of the coincidence site lattice is either equal to Σ or a submultiple of Σ, if there are additional coincidences within the larger rectangular cell. This point can be settled by inspection (stage 1).

Now it is possible to pick out such a rectangular lattice on any plane (hkl) in the cubic system. $[\overline{k^2+l^2}, hk, hl]$ and $[0l\bar{k}]$ are perpendicular directions in the plane (hkl). These directions can be used to construct a rectangular cell with the axial ratio, $\sqrt{h^2+k^2+l^2}$. It is easily established from a consideration of the area of the cell that there are (k^2+l^2-1) atoms within the unit cell, each one of which is the origin of similar rectangular cells displaced from the one illustrated.

First, Σ_R for the rectangular lattice in the basal plane is determined by the process described above. Σ_P, the multiplicity of the two-dimensional coincidence-site lattice on the basal plane, is equal either to Σ_R or to a multiple, if the rectangular lattices generated by the (k^2+l^2-1) atoms within the unit cell do not come into the same degree of coincidence. This point can be settled by inspection (stage 2). In the third step one has to consider the planes parallel to the basal plane. Σ_T, the multiplicity of the three-dimensional coincidence site lattice is either equal to Σ_P or $(h^2+k^2+l^2)\,\Sigma_P$, if the other planes in the stacking sequence do not come into the same degree of coincidence. Almost invariably it is found that Σ_T so derived is equal to Σ as given by the formula $\Sigma=x^2+R^2y^2$. This is because many of the factors tend to cancel out. It is to be hoped that later work will utilize this point to eliminate the several stages of inspection. Until then this method can serve for a systematic derivation of coincidence site lattice.

As Σ has odd values only in the cubic system (Friedel, 1926), it is necessary to devide the even values of Σ by multiples of two to obtain the correct multiplicity. From the generating function $\Sigma=x^2+(h^2+k^2+l^2)y^2$, Σ values are arrived at by a systematic assignment of integer values for x and y. The criterion of visibility introduced above (see *Previous work*) then demands that x and y should be relatively prime, *i.e.* have no common divisors except one. This merely means that it is not necessary to consider points with coordinates

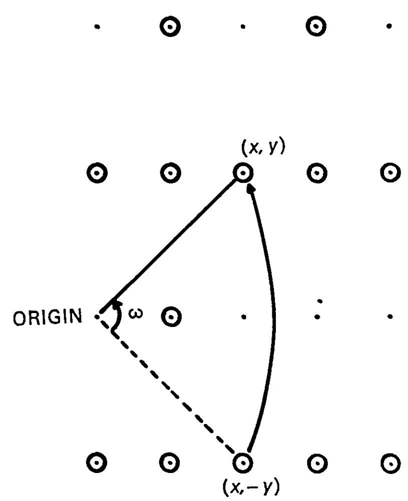

Fig. 1. Construction of a coincidence-site lattice in a rectangular lattice. Visible points are circles.

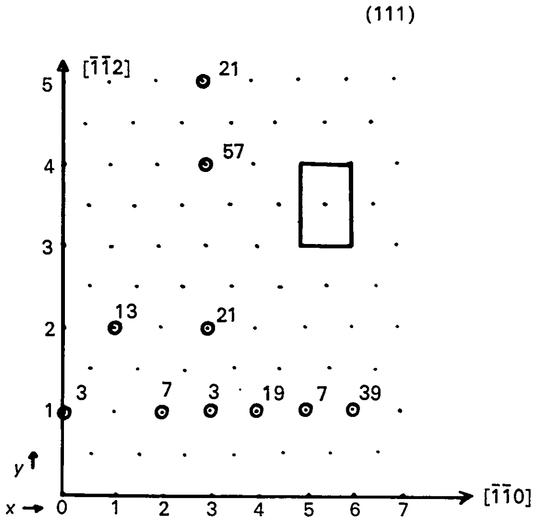

Fig. 2. This diagram illustrates the use of the generating function $\Sigma=x^2+3y^2$ for [111] rotations. The visible points are marked with the appropriate multiplicity numbers. The method of representation follows that of Dunn & Brandhorst (1958).

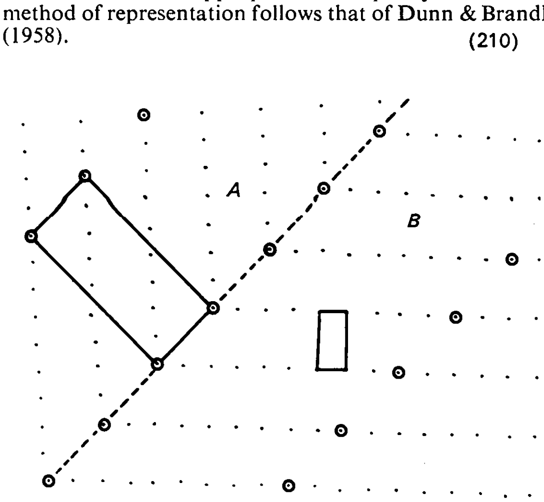

Fig. 3. Coincidence-site lattice (with $\Sigma=9$) based on [210].

(nx, ny) as they generate the same coincidence site lattice as point (x, y).

We will now illustrate the method with reference to the axis [111]. Fig. 2 shows the basal plane (111) in a f.c.c. lattice. The rectangular unit cell is marked.

Fig. 3 gives the coincidence site lattice with $\Sigma = 9$ for the case of [210] in b.c.c. Table 2 gives a list of Σ values arrived at by this method.

It is worth noting that the generating function developed here applies to the cubic system and hence has equal validity in the three cubic lattices. (This is clear since the formula for the multiplicity values involves only the indices of the axis.) An equivalent statement is that Σ and ω values are the same for a given axis in all the three lattices.

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Table 1. *Coincidence site lattice relationships for* [111]

$\Sigma = x^2 + 3y^2$ $\omega = 2 \tan^{-1} \frac{y}{x} . \sqrt{3}$

x	y	Σ	ω
0	1	3	180°
1	1	1 (=4/4)	120
2	1	7	81·8
3	1	3 (=12/4)	60
4	1	19	46·8
5	1	7 (=28/4)	38·2
6	1	39	32·2
x	y	Σ	ω
1	0	1	0°
3	1	3 (=12/4)	60
3	2	21	98·2
1	1	1 (=4/4)	120
3	4	57	133·2
3	5	21 (=84/4)	141·8
1	2	13	147·8

Table 2. *Coincidence site lattice relationships for* [210]

$\Sigma = x^2 + 5y^2$ $\omega = 2 \tan^{-1} \frac{y}{x} . \sqrt{5}$

A

x	y	Σ	ω
0	1	5	180°
1	1	3 (=6/2)	131·8
2	1	9	96·4
3	1	7 (=14/2)	73·4
4	1	21	58·4
5	1	15 (=30/2)	48·2

B

x	y	Σ	ω
1	0	1	0°
5	1	15 (=30/2)	48·2
5	2	45	83·6
5	3	35 (=70/2)	106·6
5	4	105	121·6
1	1	3 (=6/2)	131·8

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