102. *Studies in the Lattice Analysis. I*

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A crystal is, when it is subjected to the change of environment, transformed into another form usually with different symmetry. In case the original crystal possesses a number of crystallographically equivalent directions, twinning takes place about them simultaneously at its different parts. This would give rise to the domains which have different but definite orientations mutually. Such a domain scatters the x-rays incoherently to the other domains. The resulting x-ray pattern will be a composite one with all the reflections from each domain superimposed.

The lattice analysis purports to resolve the composite pattern into those due to the individual domains and to arrive at the ultimate lattice underlying the domain structure. In the course of analysis the mutual orientation of domains and also that with respect to the original lattice shall be worked out. The lattice analysis is indeed an indispensable step that should precede always the structure analysis of a domain crystal.

To derive a general inductive method that is immediately applicable to experimental data is extremely difficult if not impossible, the appropriate procedure being variable according to circumstances. In the simplest case a cubic complex (we now call so the domain structure originated from a cubic lattice) is often the compound of lattices retaining in themselves units inherited from the original lattice and the lowering of their symmetry is due to repeated twinning, generally gliding. The x-ray pattern obtained therefrom will exhibit peculiar features easy to discern and will present a typical

Fig. 1. Superlattice of a cubic unit due to regularly repeated gliding along [001] on (010).

example for the use of lattice analysis. Although we know so far only a few examples of such a complex it seems to be worth while to elaborate the method to be adopted.

The cubic complex is, as already assumed, a domain structure, each of which contains a superlattice of the original cubic unit, the

Fig. 2. Reciprocal representation of superlattices of a cubic unit due to gliding. Fig. (a) corresponds to the superlattice given in Fig. 1, and (g) is the final representation of the cubic complex derived by the synthesis of (a)–(f). Large dots and small ones show main reflections and satellites respectively, and the numbers each associated with each of the satellites in (g) indicate weight.

mechanism of superposition having been named G^1 (en echelon), G^2 (alternate), or G^3 (complex) (Ito, 1950). Let the direction and separation of gliding be along $[001]$ on (010) and the multiple of the $b(=a)$ respectively (Fig. 1). A superlattice will then appear along the b^* of the diffraction pattern. We now take into account only these lines nearest to each of the main reflections (due to the original cubic units) and name them their satellites. Now that the direction of gliding is $[001]$ the projection of the twinned lattice on to (001) is exactly identical with that of the original cubic lattice. The reciprocal lattice of the twinned lattice will be such as shown in Fig. 2(a). Since, however, there is no crystallographic distinction between (010) and (100) in the cubic lattice, a domain in which gliding occurs on (100) will be similar to that on (010) , giving the reciprocal lattice as shown in Fig. 2(b). The same assumption applies to the other direction of gliding (Fig. 2(c), (d), (e) and (f)). The final reciprocal representation of the cubic complex is shown in Fig. 2(g) and is the synthesis of the above (a) to (f). In this we see that 100, 010 and 001 are each accompanied by satellites with single weight, 110, 011 and 101 each by six satellites, four of which with single weight and the remaining two with double weight, and 111 by six satellites with double weight.

The way in which we, as illustrated above, transcribed the cubic complex into its reciprocal lattice, is not so simple as it seems at a glance when we go on to find out satellites in the neighbourhood of general hko or hkl reflections as it requires extended perspective drawings. Therefore we made, instead, use of the stereographic projection in order to look exhaustively for the possible groups of satellites around each main reflection.

The result is shown in Fig. 3, in which the directions and planes are represented on a stereogram, Fig. 3(a)–(g) corresponding to Fig. 2(a)–(g). From these the two rules, governing the procedure, have been obtained as follows:

- (1) Satellites appear only along such a reciprocal row that is perpendicular to the plane of gliding.
- (2) The presence of gliding is detectable neither on a reciprocal net plane nor on a reciprocal row that passes the origin of the reciprocal lattice and is perpendicular to the direction of gliding. In other words no satellite due to gliding is associated with any of the main reflection on such a plane or along such a row that passes the origin of the reciprocal lattice and is perpendicular to the direction of gliding.

The two rules enables us to discover the distribution of satellites around each main reflection and conversely to verify, referring to

Fig. 3. Stereographic representation of the distribution of satellites.

Fig. (a)–(g) correspond to those in Fig. 2 respectively.

experimental findings, the existence of a certain mode of gliding as the origin of superlattices.

Reference

Ito, T. (1950): X-Ray Studies on Polymorphism. Maruzen, Tokyo.