THE GNOMONIC PROJECTION IN THE HEXAGONAL SYSTEM

LEWIS S. RAMSDELL,
University of Michigan, Ann Arbor, Michigan.

ABSTRACT

The implications of the alternative settings G_1 and G_2 used in the gnomonic projections of hexagonal crystals are made clear by constructing the unit cells from which the two projections are derived. This process reveals that G_1 is based on a simple hexagonal unit cell, in conventional orientation, and with the usual axial ratio. G_2 is based on a triple cell, not in the conventional orientation, and with a different axial ratio. This situation, especially with reference to the axial ratios, has not been generally recognized in the past. The G_2 setting has been commonly used for rhombohedral crystals, but the triple cell on which it is based has no direct relationship to the actual rhombohedral cell. It is concluded that there is no reason for the continued use of the G_2 setting, either for hexagonal or rhombohedral crystals.

There has arisen much confusion in the use of two-circle goniometric measurements and gnomonic projections of hexagonal crystals, largely because of the alternative settings, which were designated by Goldschmidt as G_1 and G_2, respectively. This confusion has been especially noticeable in the determination of the axial ratio for the G_1 setting, and in the derivation of the Bravais indices from the G_2 symbols.[1] It is the purpose of this paper to re-examine the gnomonic projection in these two settings, and to see if any clarification is possible.

In the usual procedure, the gnomonic projection is constructed from measurements made on an actual crystal. It can equally well be constructed from the measurements of a unit cell. For our present purpose it is necessary to reverse this latter procedure. We wish to reconstruct the unit cells upon which the G_1 and the G_2 projections are based. By doing this, the implications of the two settings are made much more evident.

This reversed procedure could be carried out directly from the gnomonic projection, but can be done more easily by using the very closely related reciprocal lattice. In order to establish the unit cell, the vertical boundary planes must be located. But they are parallel to the vertical axis, and their face-poles do not appear in the gnomonic projection. They do appear, however, in the reciprocal lattice, and can be used to locate the unit cell boundaries. The transformation from a gnomonic projection to a reciprocal lattice is very simple, and depends upon the following relationships.

Both the reciprocal lattice and the gnomonic projection are con-

[1] Palache, C., *Am. Mineral.*, **5,** 143 (1930).
Parsons, A. L., *Am. Mineral.*, **22,** 581 (1937).
Peacock, M. A., *Am. Mineral.*, **23,** 315 (1938).

structed by extending lines from the center of the crystal perpendicular to the crystal planes. In the gnomonic projection all of these lines terminate in the projection plane, giving a two-dimensional array of points. In the reciprocal lattice each line extends a distance which is the reciprocal of the interplanar spacing of the set of planes in question, thus giving a three-dimensional array of points. These points lie in horizontal levels, designated as 0, 1, 2, 3, etc. For a crystal with a simple lattice, the pattern of points in the successive levels is the same, and their respective symbols *hk* are alike, while *l* varies with the level.

The points of a gnomonic projection which represent planes with indices *hk*1 form the basic network of the projection, and have Goldschmidt symbols *pq* which are integers, with $p=h$ and $q=k$. The *hk*0 planes appear only as direction lines, while all planes *hk*2, *hk*3, etc., appear as points between the nodes of the basic network, and at least one of the symbols *pq* is a fraction.

The pattern of this basic network is identical in design with the pattern of any level of the reciprocal lattice of a crystal with a simple lattice cell.[2] Accordingly this basic network of the gnomonic projection can be used to represent any level of the reciprocal lattice by merely changing the Goldschmidt symbols *pq* (integers) to the reciprocal lattice symbol *hkl*, where $h=p$, $k=q$, and *l* is the particular level desired. Thus it is possible to go directly from the gnomonic projection of the hexagonal system to the 0-level of the reciprocal lattice (Fig. 1).

The two projections, G_1 and G_2, as defined by Goldschmidt, are illustrated in Fig. 1*a*. The face poles 10 and 11 of G_1 become $\underline{11}$ and $\underline{03}$ in G_2. The face pole $\underline{01}$ of G_2, if present in G_1, would be $\frac{1}{3}\frac{1}{3}$. In these projections the last index, *l*, is of course equal to 1. If each point in Fig. 1*a* is considered to have a last index of 0 rather than 1, it can equally well represent the 0-level of the reciprocal lattice. This is illustrated in Fig. 1*b*, where the 0-levels of the reciprocal lattices corresponding to the G_1 and G_2 settings are shown.

The distance in the 0-level from any point to the origin is the reciprocal of the spacing of the set of planes represented by that point. By arbitrarily choosing a reciprocal factor, we can reconstruct the unit cells on which

[2] In centered lattices, because of characteristic absences, successive levels of the reciprocal lattice are different. In non-orthogonal crystals successive levels may have the same pattern, but are shifted horizontally. The above statement says the pattern of the basic projection network is identical in design with that of any level of the reciprocal lattice for a crystal based on a simple lattice. The actual size of the two networks depends upon arbitrary factors. Thus the size of the gnomonic projection network depends upon the radius of the unit sphere, which is usually chosen as 5 cm. The actual size of the reciprocal lattice network can be made identical with that of the projection by an appropriate choice of the reciprocal factor.

the two projections G_1 and G_2 are based. This is shown in Fig. 2. The small unit cell $OABC$ is derived from the larger reciprocal lattice unit $ODEF$ (G_1), while the large unit cell $OLMN$ is derived from the smaller lattice unit $ORDS$ (G_2). Thus it is evident that the G_1 projection is based on a simple hexagonal unit cell, $OABC$, and that G_2 is based on a multiple cell $OLMN$, whose cross-section is three times that of $OABC$. The cell $OABC$ has its primitive translation a_0^1 in the usual secondary position, while $OLMN$ has its primitive translation a_0^2 in the intermediate position. Both cells have the same vertical translation c_0.

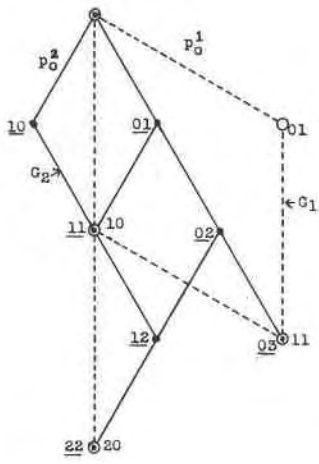

FIG. 1*a*

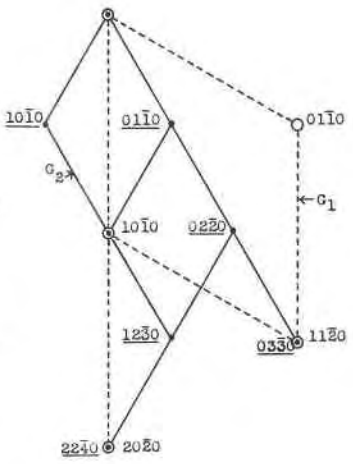

FIG. 1*b*

FIG. 1*a*. Gnomonic projections of the hexagonal system in the two settings, G_1 and G_2. G_1 is shown in dashed lines; G_2 is in solid lines and the G_2 symbols are underscored.

FIG. 1*b*. 0-level reciprocal lattices derived from the two gnomonic projections of Fig. 1*a*.

The axial ratio for the simple cell $OABC$ is $c^1=c_0/a_0^1$. This is the value which would be derived from goniometric measurements in the conventional orientation, hence $c^1=c$. Thus in Fig. 1*a* the distance p_0^1 is equal to $c_0/a_0^1\sqrt{\frac{3}{4}}$, hence $p_0^1\times\sqrt{\frac{3}{4}}=c^1=c$. For the triple cell the axial ratio is $c_0/a_0^2=c^2=c/\sqrt{3}$, and in Fig. 1*a* the distance $p_0^2=c_0/a_0^2\sqrt{\frac{3}{4}}$, and $p_0^2\times\sqrt{\frac{3}{4}}=c^2=c/\sqrt{3}$. But in terms of the true unit cell $p_0^2=c_0/a_0^1 3/2$, and $p_0^2\times 3/2=c$.

For crystals based upon a rhombohedral unit cell exactly the same relationships exist. If the rhombohedral cell is referred to hexagonal axes, new points are added at $\frac{1}{3}\frac{2}{3}\frac{2}{3}$ and $\frac{2}{3}\frac{1}{3}\frac{1}{3}$ in the simple cell $OABC$, and corresponding points in the triple cell, but the cell outlines remain unchanged, as do the geometrical relationships involving c^1, c^2 and c, namely $c^1=c$ and $c^2=c/\sqrt{3}$.

These relationships differ from those derived by Goldschmidt.[3] His equations relating G_1 and G_2 to c are the same as above, but he introduced values of c^1 and c^2 as follows:

$$(G_1)\ p_0{}^1 \times 3/2 = c^1 = c\sqrt{3}.\ (G_2)\ p_0{}^2 \times 3/2 = c^2 = c.$$

These values of c^1 and c^2 are such that the length of a, taken as unity in the G_1 cell, must be equal to the distance OH (Fig. 2), and in the G_2 cell equal to the distance OA. Obviously OH is less than unity in the cell $OABC$, and hence his value of c^1 is too large; $c^1 = c\sqrt{3}$. It so happens that OA, which is not equal to unity in the triple cell, is equal to unity in the G_1 cell, and hence Goldschmidt's value of c^2 is incorrect for G_2 but correct

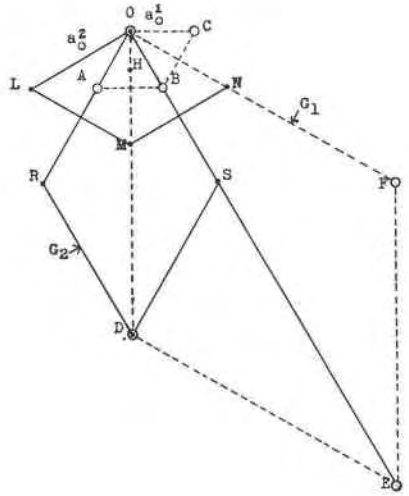

FIG. 2. 0-level reciprocal lattices for the G_1 and G_2 settings, with the unit cells upon which they are based. The small G_1 unit cell $OABC$ (dashed lines) gives rise to the large reciprocal lattice unit $ODEF$ (dashed lines). The triple G_2 unit cell $OLMN$ gives rise to the small reciprocal lattice unit $ORDS$.

for G_1, and thus his value of c^2 agrees with the customary value of c. This situation results from the fact that although the axial ratio was derived from $11\bar{2}1$, which cuts at unity on two secondary axes 120° apart, he used the intercepts of this face on the two intermediate axes 60° apart for his unit values in determining c^1 and c^2.

The G_1 setting has commonly been used for crystals with hexagonal development, and as used by Goldschmidt did not give the proper value of c. The G_2 setting has been considered more suitable for crystals with a rhombohedral development. As has been shown, the G_1 setting is based

[3] Goldschmidt, V., Index der Krystallformen der Mineralien, vol. 1, 33–35 (1886).

on a simple hexagonal unit cell in the customary orientation, and its symbols correspond to the usual Bravais indices. The objection that it does not give the correct value of c has no validity. On the other hand, the G_2 setting is based on a triple cell, with a value of c different from the customary one, although this fact has not been generally recognized in the past.

Actually this triple cell is sometimes used in crystal structure descriptions. In certain symmetry groups of the hexagonal system the secondary and intermediate positions do not carry the same symmetry elements, and are therefore distinguishable. For example, in the ditrigonal pyramidal class there are three vertical symmetry planes, and in the usual morphological description of this class, these planes are considered as being in the intermediate positions. But structurally the alternative arrangement, with three planes in the secondary positions, is equally possible, hence the two space groups $C3m1$ and $C31m$. To bring the structural data in harmony with the morphological data in this latter case, the triple cell may be used, for it reverses the intermediate and secondary positions. This convention, however, has no application to rhombohedral crystals, which are always described either in terms of rhombohedral axes, or else in terms of the unit hexagonal cell of the G_1 setting.

The question thus arises as to whether there is any good reason for continuing the use of the G_2 projection. A possible advantage is that it has three times as many nodes in its basic network, and therefore has three times as many possible face-poles for which the Goldschmidt symbols will be integers. This would apply equally to both hexagonal and rhombohedral crystals. Of more significance is the fact that the most prominent $hk\bar{i}l$ zones in rhombohedral crystals coincide with the basic network of G_2 rather than G_1, so that at least one of the Goldschmidt G_2 symbols is an integer, and is common to all faces of the zone.

It would seem that this slight advantage is greatly outweighed by the confusion caused by a dual system, with two orientations, two sets of symbols and indices, and two axial ratios. It is therefore concluded that there is no sufficient reason for retaining the G_2 projection, and that in the future all hexagonal crystals, both with hexagonal and rhombohedral developments, should be described in terms of the G_1 projection.

ACKNOWLEDGMENT

The writer is indebted to Professor M. A. Peacock, of the University of Toronto, who kindly read an early draft of this paper and made several helpful suggestions, and who also heartily concurred in the conclusion that the G_2 projection should be dropped.