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Atomic arrangements on the twin boundaries of crystals of calcite and aragonite

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ABSTRACT. By constructing ball-and-spoke models an attempt has been made to arrive at the atomic arrangements on the twin boundaries of four twins of calcite and one of aragonite. The Miller indices of the twins of calcite are (111), (110), (100) and (11$\bar{1}$). The twin plane in aragonite is (110). Each of the models of calcite twins has the same plane for twin plane and composition plane, and in each case it is a true mirror plane. Aragonite has a pseudo glide plane parallel to (110) gliding in the [001] direction. By making this pseudo symmetry element into a true glide plane a good model of the twin is obtained. In the (111), (110) and (100) twins of calcite all the CO_3 groups in the composition plane are parallel to it. In the (11$\bar{1}$) twin the composition plane contains only CO_3 groups and these are perpendicular to it.

AT present it is hardly possible to study experimentally the actual atomic arrangements at twin boundaries of calcite and aragonite. The method which has been adopted here is to construct, with balls and spokes, scale models of the various twins, always following certain rules. The interatomic distances have been made, as nearly as possible, the same as in the single crystals.

Calcite

Calcite has four types of twin, having Miller indices (111), (100), (110) and (11$\bar{1}$) referred to the usual rhombohedral axes, which are parallel to edges of the cleavage rhombohedron. In the crystal structure there is a corresponding pseudo unit cell having $a = 6.41$ Å and $\alpha = 101°\ 55'$. The twin planes have Bravais-Miller indices (0001), (10$\bar{1}$1), (01$\bar{1}$2) and (02$\bar{2}$1) respectively when referred to the hexagonal unit cell derived from the rhombohedral cell given above.

Twin plane (111), (0001). The twin on plane (111) is illustrated in fig. 1, both in terms of the atomic positions and the external faces of the twin. In this model the twin plane is a mirror plane of symmetry so that the atoms marked A, B occur on a line perpendicular to the twin plane. The distance between these atoms is less than normal though it is to be expected that there would be in the actual crystal some adjustment between the Ca-O distances. The coordination of these calcium atoms is shown in fig. 6.

Twin plane (100), (10$\bar{1}\bar{1}$). The twin on plane (100) is shown in fig. 2. In this model the twin plane is a mirror plane of symmetry. Two of the Ca-O distances are somewhat shorter than the rest in the twin plane—2.1 as compared with 2.35 Å. The plane of the CO_3 group coincides with the twin composition plane. On either side of the composition plane the CO_3 groups are inclined at an angle of $45\frac{1}{2}°$

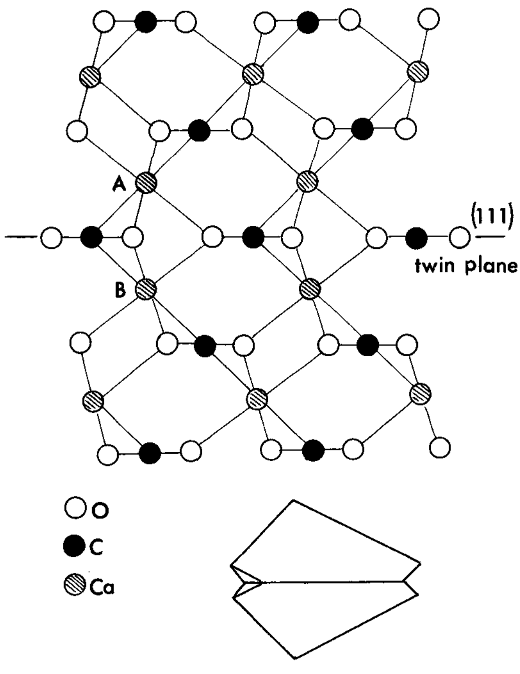

FIG. 1. Projection of atoms in (111) twin of calcite on to a plane containing the [111] direction. Inset: Drawing of the natural twin.

to the twin plane. In the composition plane one oxygen of each CO_3 group is joined to two calcium atoms (as in the single crystal), a second oxygen is joined to three calcium atoms by long bonds, and the third oxygen is joined by a short bond to only one calcium. The coordination of the calcium atoms is sixfold as in the single crystal.

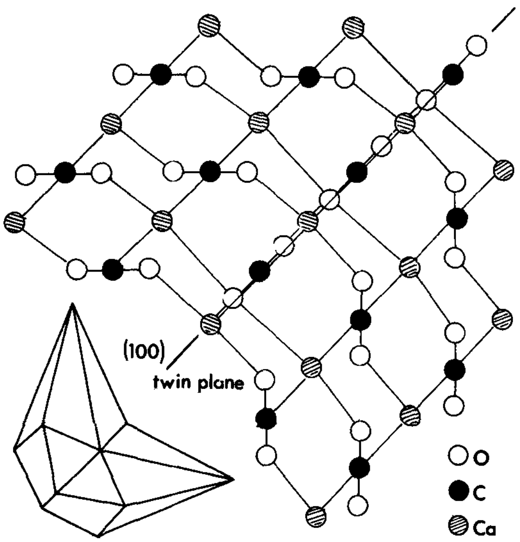

FIG. 2. Projection of atoms in (100) twin of calcite on to a plane containing the [111] axes of both parts of the twin. Inset: Drawing of the natural twin.

Twin plane (110), (01$\bar{1}$2). The twin plane on (110) is shown in fig. 3. The composition plane is a mirror plane of symmetry in which the CO_3 groups lie. In the composition plane the bonds to the calcium atoms are almost normal but, as in the (100) twin, the oxygens of the CO_3 group are joined to one, two, and three calciums respectively. This twin shows polysynthetic twinning often parallel to only one {110} face.

Twin plane (11$\bar{1}$), (02$\bar{2}$1). This rather rare twin is illustrated in fig. 4. The composition plane is a mirror plane of symmetry. All the CO_3 groups intersected by the composition plane lie perpendicular to it. The coordination of all the atoms is the same as in the single crystal and the interatomic distances are also almost normal.

Discussion of the calcite twins. The rhombohedral configuration shown in fig. 5 is that which occurs in the single crystal. The trigonal arrangement of fig. 6 is that which occurs in the model of the (111) twin. Figure 7 shows a possible linear arrangement of the atoms. This is close to the actual arrangement

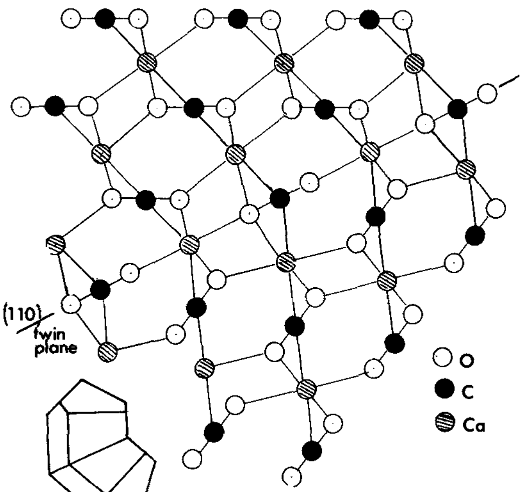

FIG. 3. Projection of atoms in (110) twin of calcite on to a plane containing the [111] axes of both parts of the twin. Inset: Drawing of the natural twin.

on the (100) face of the single crystal and is the arrangement in the composition plane of the proposed model for the (100) twin. Figure 8 shows another possible linear arrangement of the atoms. This is characteristic of the (110) twin. The twin on (11$\bar{1}$) seems to be related to the straight lines of oxygens, which occur in that face. The twin model assumes that the plane of the CO_3 groups

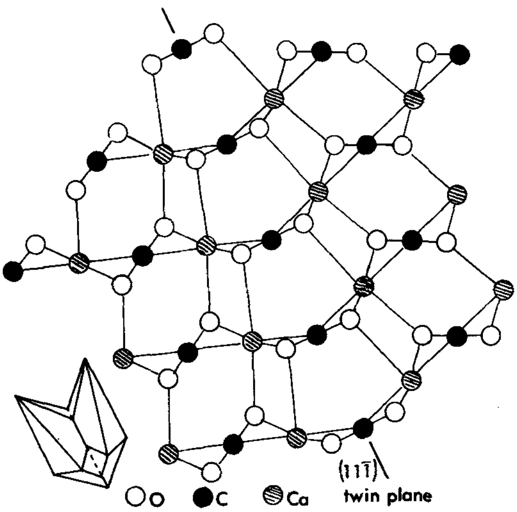

FIG. 4. Projection of atoms in (11$\bar{1}$) twin of calcite on to a plane containing the [111] axes of both parts of the twin. Inset: Drawing of the natural twin.

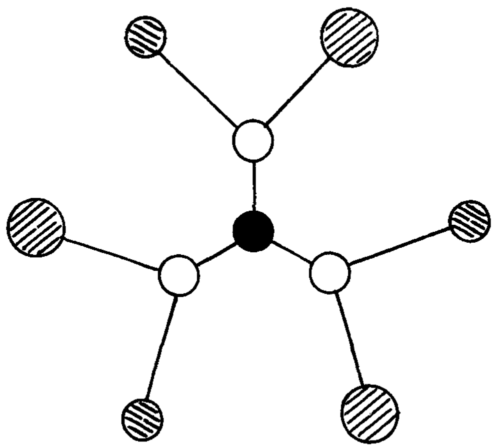

FIG. 5. The arrangement of calcium atoms about the carbonate radicals in the untwinned calcite crystal projected on to the (111) plane.

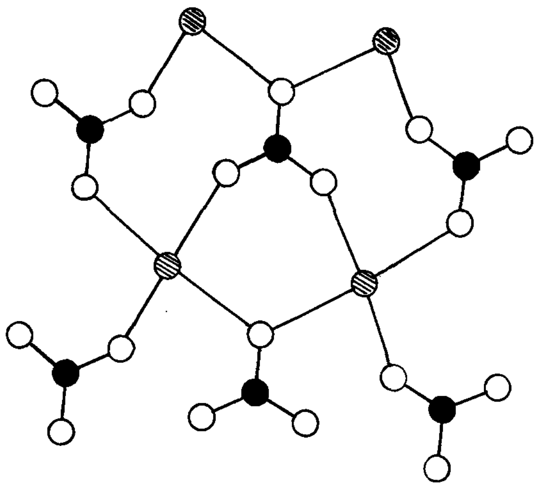

FIG. 7. The arrangement in the composition plane of calcium atoms about the carbonate radicals in the (100) twin of calcite.

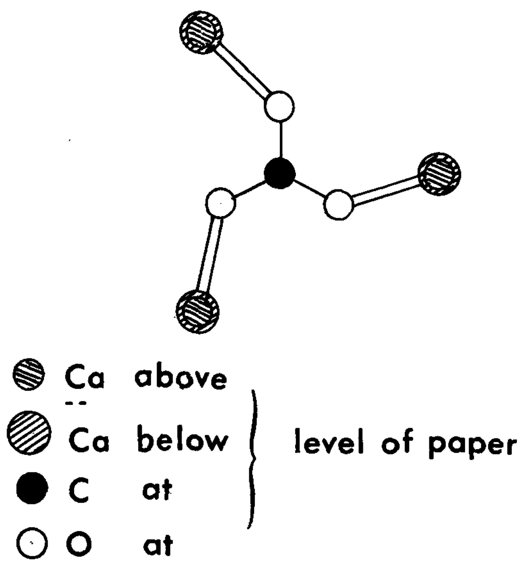

FIG. 6. The arrangement in the composition plane of calcium atoms about the carbonate radicals in the (111) twin of calcite.

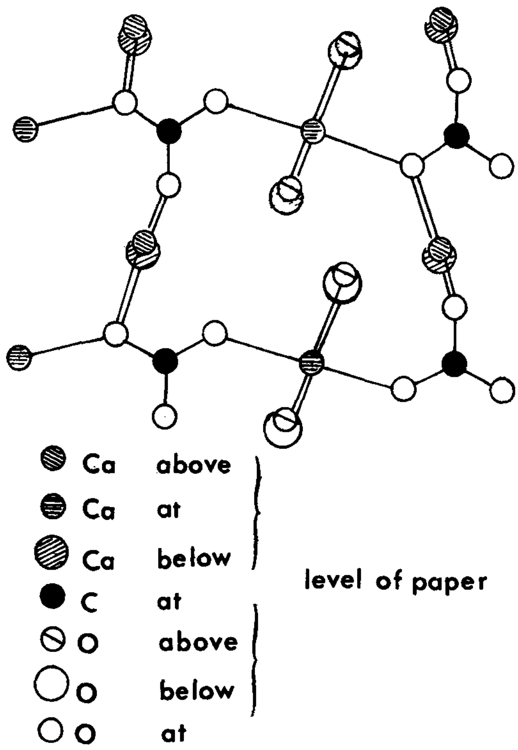

FIG. 8. The arrangement in the composition plane of calcium atoms about the carbonate radicals in the (110) twin of calcite.

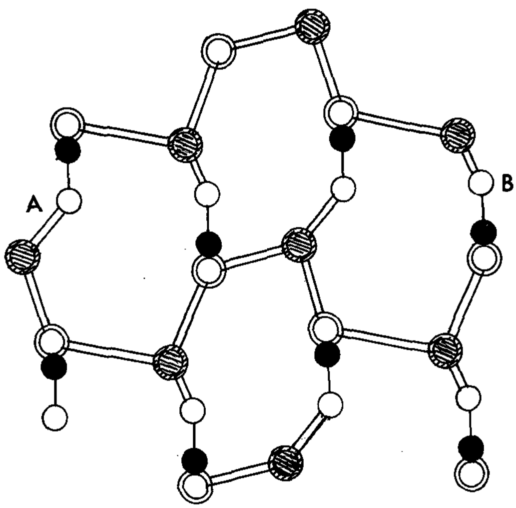

FIG. 9. The arrangement in the composition plane of calcium atoms about the carbonate radicals in the (11$\bar{1}$) twin of calcite.

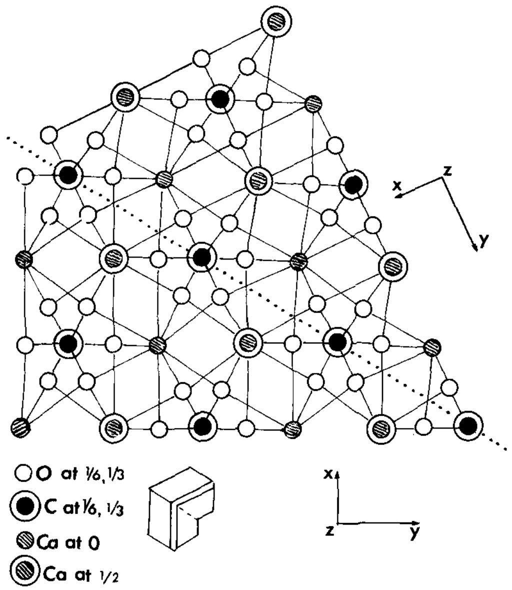

FIG. 10. Projection of atoms in the (110) twin of aragonite on to a (001) plane.

is perpendicular to these lines of oxygens, as is indicated in fig. 9. The (111) and (110) twins are often repeated and produce twin lamellae. It seems probable that this is associated with the ease with which the corresponding groupings of calcium atoms and carbonate radicals can deposit on the already grown single crystal surface. The (100) and (11$\bar{1}$) twins do not form such lamellae and appear to start growing from the single composition plane on both sides of it.

Aragonite

The crystal structure of aragonite is orthorhombic having $a = 4.94$, $b = 7.94$, $c = 5.72$ Å. The twin plane is (110) and the proposed model of the structure of the twinned crystal is shown in fig. 10. There is a pseudo glide plane parallel to (110), gliding in the [001] direction and represented by the dotted line in fig. 10. The model of the twin given here is obtained by making the pseudo into a true glide plane. It is necessary to look carefully at the model in order to observe the difference between the original and the twinned portion. The environment of all the atoms on the composition plane is very similar to that which obtains in the single crystal. This twin is often repeated, giving crystals with a pseudo-hexagonal character. This accords with the pseudo-hexagonal character of the atomic arrangement.

Bragg (1937) gives an explanation of this twin law based on the possibility of regarding some of the atoms in a section between two (110) planes as belonging equally to either half of the twin. This does not take into account the pseudo glide plane which in the twinned crystal becomes a true glide plane.

REFERENCE

Bragg, W. L. (1937) *Atomic structure of minerals.* O.U.P., London.

[*Manuscript received 18 May 1981; revised 16 September 1981*]