

SHORT COMMUNICATIONS

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Atomic arrangements on the twin boundaries of orthoclase twins

IN the extensive literature dealing with the growth twinning in crystals, two approaches have been followed. Friedel (1926) related twinning to a lattice common to both parts of the twin, while others have considered how the atoms at the junction must be packed to give substantially the same interatomic distance and bond angles as in the single crystal. The second approach has been adopted in this paper.

This investigation has been carried out by constructing ball-and-spoke models of the various twins. The balls constituting the boundary between the two parts of the twin have been drilled to accord with the full symmetry of the twinned crystal, while the rest of the model has the normal symmetry of the untwinned crystal. The orientation of the two sets of crystallographic axes is determined by the twin law. Only when it was possible to construct a model in which the environment of the boundary balls closely approximated to the normal environment, was the proposed atomic arrangement accepted.

It has been found that there are several types of composition plane required if these conditions of similar bond lengths and angles are to be fulfilled. They may conveniently be illustrated by the twin laws of orthoclase, KAlSi_3O_8 , namely, the Carlsbad, Manebach, Baveno, and X-twin. Using the parameters given by Cole *et al.* (1949), orthoclase is monoclinic, $a = 8.564$, $b = 13.03$, $c = 7.175$, $\beta = 115.994^\circ$ and belongs to the space-group $C2/m$. Fig. 1b is a projection of part of the structure on a plane normal to the $[001]$ -axis, and shows that there is a tubular arrangement of atoms running parallel to that axis. These tubes have almost orthorhombic symmetry. There is a true plane of symmetry, which is an element of the space-group, parallel to (010) passing through the axis of the tube. In addition, there is a pseudo plane of symmetry, which is parallel to (100) and is represented by the wavy line. The intersection of these planes gives rise to a pseudo diad axis along the axis of the tube. This is represented by an arrow with a small circle or an open rhombus. Fig. 2 shows a second series of tubes in the structure to which

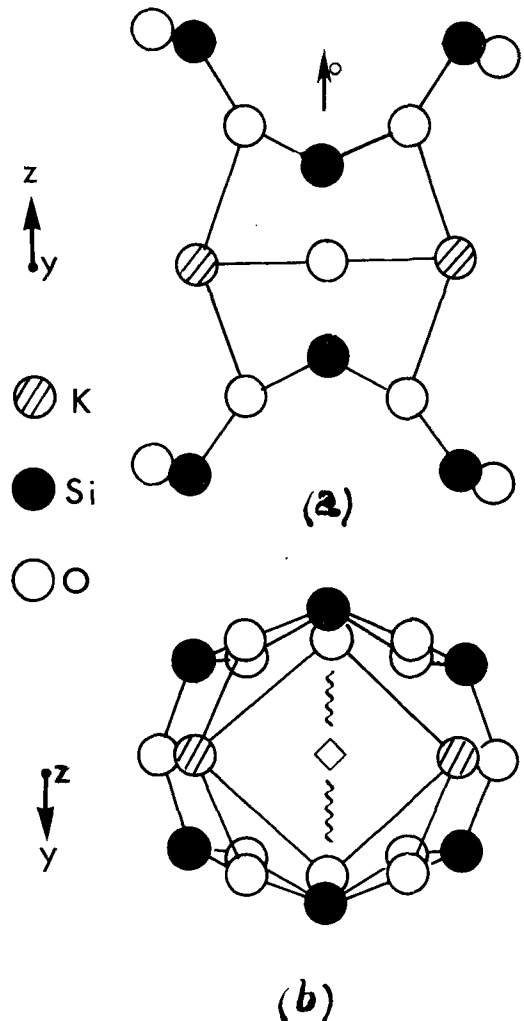


FIG. 1. (a) Projection on (010) of the tubular element in the crystal structure of orthoclase. (b) Projection on a plane normal to the $[001]$ -axis of the same structural element: \uparrow pseudo diad axis lying in the plane of the paper, $\{$ pseudo diad axis perpendicular to the plane of the paper, \diamond pseudo plane of symmetry perpendicular to the paper.

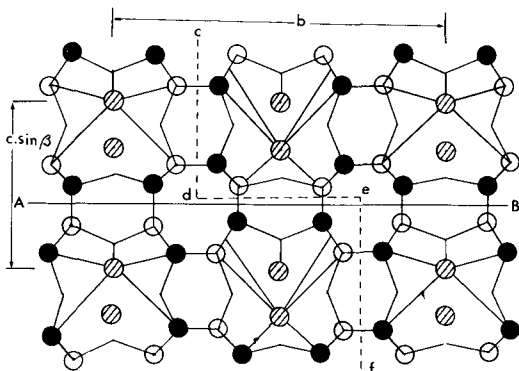


FIG. 2. Diagrammatic representation of a projection of the unit cell of orthoclase on to a plane normal to the $[100]$ -axis. AB composition plane for Manebach twin. $cdef$ composition plane for Baveno twin.

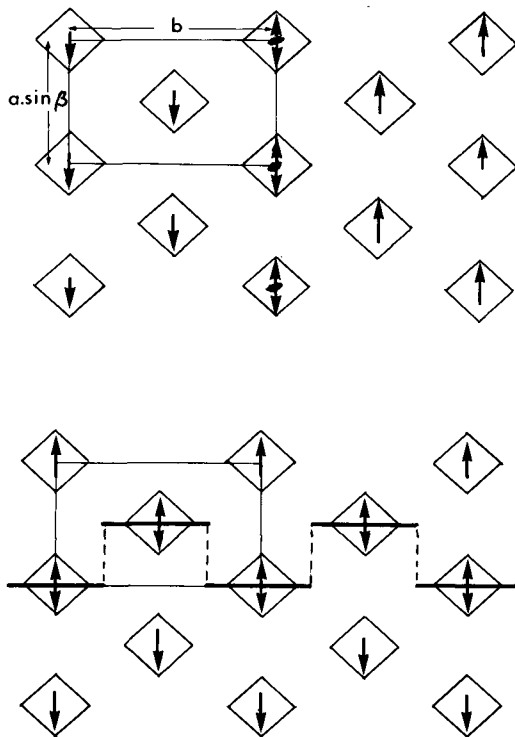
Taylor *et al.* (1934) and Bragg (1937) have drawn attention. These are almost square in section and run parallel to the $[100]$ -axis. They are represented by the twelve-sided figures containing the shaded circles, which represent the potassium atoms.

The *Carlsbad twin* is defined as having $[001]$ as the twin axis and (010) as the composition plane. The parts of the twin frequently interpenetrate so that the statement about the composition plane cannot refer to all junctions between the two parts of the twin. The twin axis is the same as the pseudo diad axis of the tubular column of atoms shown in fig. 1*b*. In fig. 3 the tubular atomic column is represented by a rhombus. On the left-hand side the arrows pointing downwards represent the direction of the positive sense of the $[100]$ -axis. In the middle the arrows pointing in both directions represent the atoms arranged with a true diad axis so that both directions of the arrow are equivalent. On the right-hand side the arrows are pointing upwards corresponding to the twin orientation.

The *X-twin* is defined by Deer *et al.* (1963) as having a twin axis perpendicular to (100) and a composition plane (100) . Since the crystal has a centre of symmetry this definition is equivalent to saying that the twin is a reflection in (100) with the same plane as the composition plane. The structural elements shown in fig. 1*a, b* have a pseudo diad axis normal to (100) but this pseudo symmetry does not extend beyond the tubular element in which it is located. It is, therefore, not possible to construct a twin on this basis. It is possible, however, to construct a model using the pseudo plane of symmetry parallel to (100) . In fig. 4 the tubular element of fig. 1 is again represented by a rhombus and the pseudo planes of symmetry by thick lines. The arrows indicate the positive direction of the

x -axis and by making the composition plane *crenellated* it is possible to have the arrows pointing in opposite directions in the upper and lower parts of fig. 4. It thus appears that on the basis of model construction the *X-twin law* should be a twin plane parallel to (100) and a crenellated composition plane also parallel to (100) .

The *Manebach twin* is defined as having the normal to (001) as the twin axis and the same plane as the composition plane. A projection of the unit cell on to a plane normal to $[100]$ is diagrammatically represented in fig. 2. Along the line AB it can be seen that all the bonds are nearly parallel to the paper, i.e. normal to (001) . Each bond joins an oxygen to a silicon and no other type of bond crosses the plane AB . On both sides of the plane of which AB is the projection the atoms next to this plane have a pseudo diad axis symmetry. In fig. 5 the atoms on the underside of the plane AB are projected on to the plane (001) . The departure of any atom from the position corresponding to diad axis symmetry does not exceed 0.3 \AA . The



FIGS. 3 and 4. FIG. 3 (top). Diagrammatic representation of the Carlsbad twin projected on to a plane normal to the $[001]$ -axis. FIG. 4 (bottom). Diagrammatic representation of the *X-twin* projected on to a plane normal to the $[001]$ -axis.

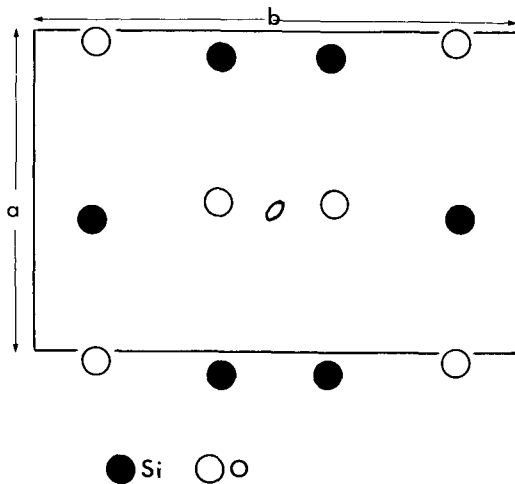


FIG. 5. Projection on to a (001)-plane of the silicon and oxygen atoms just below the line *AB* in fig. 2.

bond angles are only a little changed. Thus it is possible for the portion above the plane *AB* to be rotated about the twin axis through 180° and it then almost superposes on the positions which were occupied by the same kinds of atoms before the rotation. Bragg (1937) gave an explanation of this twin as a reflection across the plane (001). Examination of the model of the unit cell shows that if all the atoms are taken into account there is neither a pseudo reflection plane nor a pseudo glide plane parallel to (001). Thus the model requires that the twin law be a twin axis normal to (001) with the same plane as the composition plane.

The *Baveno* twin is defined as having a twin axis normal to the plane (021) and the same plane as the composition plane. Bragg (1937) had attributed this twin to a pseudo glide plane parallel to (021). In putting forward this proposal he had deliberately omitted consideration of the potassium atoms. I could not find any pseudo glide plane parallel to (021) so I sought for an explanation along the lines which had been successful with the *Manebach* twin. It was noticed that across certain planes parallel to (010) there were only Si–O bonds and that these were almost perpendicular to the (010) plane. A model of the orthoclase structure was constructed in two parts separated by the planes (010) and (001), projected as the dashed lines *cdef* in fig. 2. It was found that when the one half was

rotated through 180° about the normal to (021)—a line bisecting the angle *cde*—and the two halves of the model were put together again, every silicon came opposite an oxygen and vice versa. It is therefore concluded that the composition plane is like a *staircase* and that the twin law is a rotation of 180° about the normal to the plane (021). A staircase-type of composition plane has been described for iron pyrites (Donnay *et al.*, 1977).

Discussion. In this paper an attempt has been made to relate the mutual orientation of the two parts of several orthoclase twins to features of the crystal structure. Carlsbad twins are often interpenetrant, which may be connected with the small change in atomic positions on the tubular element described in fig. 1*b* that is required to bring the structure to the twinned orientation. The *Baveno* twin sometimes occurs as a fourling, which may be due to the fact that a (02 $\bar{1}$) plane could serve equally well as a (021) plane for the twin. The *Manebach* twin usually occurs simply with a single (001) plane as the composition plane. According to the theory advanced here there would be no easy way of forming anything except a planar twin boundary. It would seem probable that the *Manebach* twin begins as a very thin platelet parallel to (001) having diad axis symmetry in a direction normal to it. Subsequent growth on both sides of this platelet would result in the observed twin.

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