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The Peierls Force in Crystalline Quartz[1]

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Abstract

The stability of the SiO_4 tetrahedron suggests that dislocations in high- and low-quartz should be regarded as dislocations in the helical arrangements of the SiO_4 tetrahedra, the axes of which are parallel to the observed Burgers vectors. The resulting core distortions are easy to visualize for screw dislocations and provide a geometrical interpretation of the Peierls force resisting dislocation glide.

The basic structural unit common to all forms of silica is the SiO_4 tetrahedron in which a silicon atom fits interstitially between four oxygen atoms. This unit is extremely stable; it is only the spatial arrangement and precise geometry of the unit which varies from one form of silica to another. Consequently, the nature of defects such as dislocations is expected to be such that the basic unit remains more or less intact.

The Burgers vectors for the primary slip systems in high- and low-quartz (Christie and Green, 1964; Griggs and Blacic, 1965; Baëta and Ashbee, 1969) are **a**, **c**, and **a**+**c**, of which **a** and **c** are both parallel to the axes of channels defined by helical chains of SiO_4 tetrahedra joined together at their corners. These facts are illustrated in Figure 1(a) for the **a**-axis and in Figure 1(b) for the **c**-axis. There are two kinds of channel parallel to both **a** and **c**, one of whose cross-section is a hexagon and the other either a rectangle (parallel to **a**) or a triangle (parallel to **c**). The rectangular and triangular channels are defined each by a single helix with, respectively, four and three tetrahedra per pitch and of pitch equal in magnitude to the Burgers vector, so a screw dislocation along the axis of either channel changes the helix into rings of tetrahedra or into a double helix of twice pitch, depending on the sign of the Burgers vector.

The hexagonal channels parallel to **a** and **c** are each defined by a double helix with six tetrahedra per pitch and of pitch equal in magnitude to twice the modulus of the Burgers vector. Depending on the sign of the Burgers vector **b**, a screw dislocation converts the double helix either into a single helix of half pitch or into a triple helix of three halves pitch. Both these core distortions are illustrated for a right-handed double helix in Figure 2. If the screw dislocation does not thread the full length of the original double helix, it is terminated by an edge dislocation which, in physical terms, is simply the end or start of a single helix. Such a termination is shown at one end only of each of the screw dislocations illustrated in Figure 2(b) and (c). In a three-dimensional piece of quartz, the edge dislocation would extend across the slip plane normal to the Burgers vector.

The stable equilibrium positions represented by helices of zero or double pitch, and of half or three halves pitch, will persist even under an external stress until that stress exceeds a certain magnitude determined by the stability of the SiO_4 tetrahedron. Following F. C. Frank (as reported by Griggs, 1967), it is likely that the junctions between SiO_4 tetrahedra are scissioned one at a time, *i.e.*, that screw dislocations propagate by the migration, parallel to their lengths, of kinks and that the scissioning process is aided by the presence of water. If the latter postulate is true, it suggests that gliding dislocations sweep OH groups towards the free surfaces and that subsequent deformation requires re-diffusion of the OH groups back into the crystal. However, since the hexagonal **a** and **c** channels are so open, it is unlikely that OH diffusion is sufficiently difficult for it to dominate the Peierls force. Even if water is plentiful, dislocations in crystalline quartz would prob-

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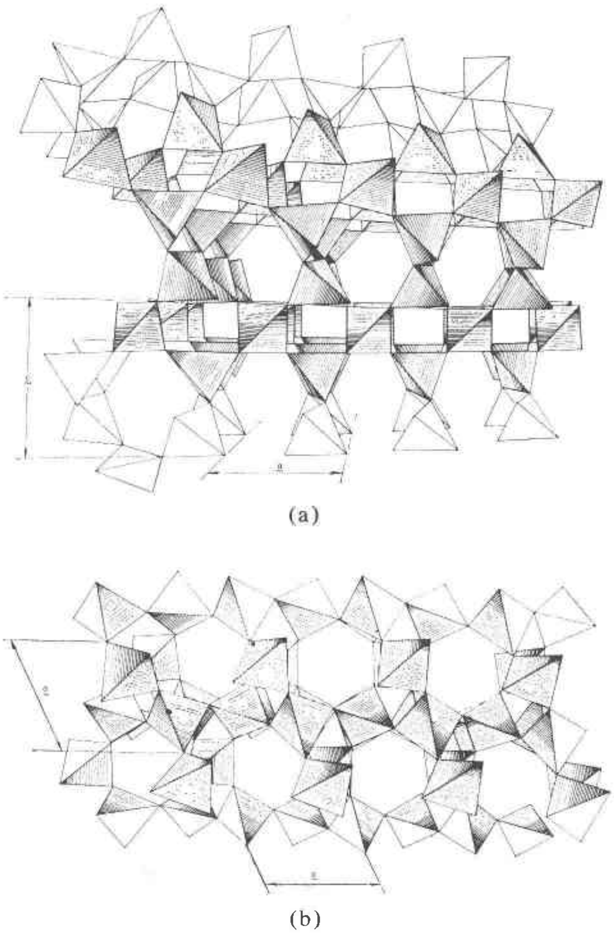

FIG. 1. Structure of morphologically right-handed high-quartz ($P6_422$). (a) Viewed parallel to **a**. (b) Viewed parallel to **c**. In low-quartz, the SiO_4 tetrahedra are slightly rotated away from the high-quartz positions in such a way as to destroy one set of two-fold axes.

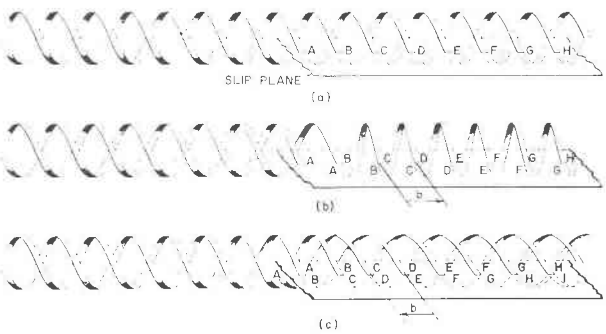

FIG. 2. (a) To introduce a screw dislocation along the axis of a high-quartz double helix, let the individual helices be scissioned at the points labelled A, B, C, *etc.* (b) With that part of the double helix above the slip plane held fixed in space, let the part below the slip plane be sheared to the right by a displacement equal to the Burgers vector **b**. (c) The dislocation introduced into (a) by a shear that is equal and opposite to that shown in (b). [Note: Some elastic relaxation from the configurations shown in (b) and (c) is expected, especially near the edge dislocations.]

ably have a high Peierls force determined by the variation of elastic energy with position. In this respect low-quartz, with its irregular SiO_4 tetrahedra and asymmetric screw dislocation cores, will be even less able to keep its energy small during glide and is expected to be characterized by a higher Peierls force than high-quartz.

Note Added in Proof

Since writing this article, the author's attention has been drawn (Harris, 1973) to the fact that the protein molecules in polymerized protein from tobacco mosaic virus occur as rings, as single helices, and as double helices, and that the observed coexistences of any two of these forms have been attributed to the presence of dislocations. Since dislocations are possible in any periodic structure, this is a plausible thesis and may also be responsible for other oddities in helical structures. However, it should be noted that, whereas the axial distance between the coaxial helices of SiO_4 tetrahedra equals half the lead (or pitch) of the helices in β-quartz and that, as a consequence, introduction of an axial screw dislocation does not impair helix continuity, this may not be so in other helical structures.

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