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SLIP SYSTEMS IN QUARTZ: II. INTERPRETATION

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ABSTRACT

Estimates have been made using linear anisotropic elasticity theory of both the non-core energy and the "ease of slip" for several basal and prismatic dislocations in high-quartz.

The influence of the crystal structure on slip is discussed, and the criterion for basal and/or prismatic slip is considered in relation to some measurements of the critical resolved shear stress for slip. It is suggested that the slip direction is more important than the slip plane in deciding the choice of glide parameters in quartz.

INTRODUCTION

The elastic constants of a crystal are described by the components of a fourth rank tensor. Consequently, the elastic behaviour is generally anisotropic; the degree of anisotropy decreases with increasing degree of crystal symmetry. High-quartz belongs to the hexagonal trapezohedral crystal class, for which the matrix of non-vanishing components of the stiffness constants is

$$\begin{vmatrix} c_{11} & c_{12} & c_{13} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{13} & 0 & 0 & 0 \\ c_{13} & c_{13} & c_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \frac{1}{2}(c_{11} - c_{12}) \end{vmatrix}$$

It is evident, therefore, that the linear parts of the elastic distortions around dislocations in quartz need to be formalised in terms of anisotropic elasticity theory.

In the present work, anisotropic elasticity theory is applied to dislocations in the quartz structure, and the criteria for basal and/or prismatic slip are investigated.

The influence of directional bonding in quartz on the choice of glide parameters is also examined, and experiments are reported of some measurements of the critical resolved shear stress for slip.

DISLOCATION ENERGIES

Foreman (1955) has shown that in an elastically anisotropic crystal, the non-core elastic energy, per unit length of a long-straight dislocation, is given by

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$$E = \frac{b^2}{4\pi}\left(\ln \frac{R}{r_0}\right) K \tag{1}$$

where b is the magnitude of the Burgers vector, R is the radius of the dislocation strain field, and r_0 is the radius of the core of the dislocation. K is an energy factor, which is a function of the elastic constants of the crystal and of the orientation of both the Burgers vector and the dislocation line.

In general, the energy factor K is obtained numerically by finding six complex parameters, which are the roots of a sextic equation (Eshelby *et al.*, 1953). However, analytical solutions for K exist for certain dislocation orientations in crystals of high symmetry. For example, in the case of a hexagonal crystal, the conditions for vanishing interactions of the separate component energies of a dislocation are satisfied if the latter is both parallel to a symmetry axis, and perpendicular to a symmetry plane. The solutions so derived by Foreman (1955) are, for an edge dislocation

$$K_e = (c_{11} + c'_{12})\left[\frac{c'_{66}(\bar{c}_{11} - c'_{12})}{c'_{22}(\bar{c}_{11} + c'_{12} + 2c'_{66})}\right]^{1/2} \tag{2}$$

and for a screw dislocation

$$K_s = (c'_{44}c'_{55})^{1/2} \tag{3}$$

where

$$\bar{c}_{11} = (c'_{11}c'_{22})^{1/2} \tag{4}$$

The C'_{ij} in equations (2)–(4) refer to axes defined in a right-handed orthogonal co-ordinate system, in which the dislocation line is parallel to the Z-axis, and the slip plane is normal to the Y-axis.

Since the crystal structure of high-quartz is hexagonal, equations (2) and (3) can be used to calculate the energy factors for dislocations of the slip systems (0001) $<\bar{1}\bar{1}20>$; $\{1\bar{1}00\}$ $<\bar{1}\bar{1}20>$, and $\{hk0\}$ [0001]. Furthermore, since the elastic constants of quartz are invariant for rotations about the C-axis, the energy factor for a mixed dislocation in the basal plane can also be calculated from the isotropic relation (Foreman 1955)

$$K_{\text{mixed}} = K_e \sin^2\theta + K_s \cos^2\theta \tag{5}$$

where θ is the angle between the slip vector and the dislocation line.

The energy factors K of various straight dislocation lines lying in the basal and prismatic planes of high-quartz were calculated using equations (2) and (3), and are given in Table 1. The values of the elastic constants of quartz assumed in these calculations are taken from the work of

TABLE 1. ELASTIC PROPERTIES OF DISLOCATIONS IN HIGH-QUARTZ

Slip system	a_{ij}	$K(\times 10^{11}$dynes/cm$^2)$	$[E/\log(R/r_0)]$ ergs/cm	ξ
(0001)	1 0 0	Pure screw 4.34	8.71	
$\langle 11\bar{2}0\rangle$	0 0 1	Pure edge 5.42	10.87	0.27 $\lvert a\rvert$
	0 −1 0	Mixed (30°) 4.61	9.24	0.23 $\lvert a\rvert$
$\{1\bar{1}00\}$	1 0 0	Pure screw 4.34	8.71	
$\langle 11\bar{2}0\rangle$	0 1 0			
	0 0 1	Pure edge 6.20	12.43	0.53 $\lvert a\rvert$
$\{1\bar{1}00\}$	0 0 −1	Pure screw 3.70	8.84	
[0001]	−1 0 0			
	0 1 0	Pure edge 5.21	12.44	0.41 $\lvert c\rvert$
$\{11\bar{2}0\}$	0 0 −1	Pure screw 3.70	8.84	
[0001]	−1 0 0			
	0 1 0	Pure edge 5.21	12.44	0.23 $\lvert c\rvert$

Kammer *et al.* (1948) and are listed in Table 2. Since these c_{ij} were measured with respect to the crystal axes used in paper I, it was necessary to transform axes to those used above to define dislocation orientations; the direction cosines a_{ij} for the co-ordinate transformation for each slip system are given in Table 1. In order to make true comparisons of the dislocation line energies, values for r_0 in equation (1) must be assumed. However, if variations of core radius are ignored, the magnitude of $E/ln(R/r_0)$, tabulated in column 4 of Table 1, may be used as measures of the respective energies. The value of $|\boldsymbol{b}|$ used to calculate E were $|\boldsymbol{a}| = 5.02$Å and $|\boldsymbol{c}| = 5.48$ Å (Frondel, 1962).

It is evident from Table 1 that, on any of the slip planes considered, the non-core elastic strain energy of a stationary dislocation is significantly lower for screw than for edge orientation. Furthermore, the energy of a mixed basal dislocation with a 30° screw component is less than that of a pure edge dislocation in the same plane. This no doubt explains the observation by McLaren *et al.* (1967) that basal dislocations in natural quartz specimens deformed by Christie *et al* (1964) under hydrostatic

TABLE 2. ELASTIC STIFFNESS CONSTANTS OF HIGH-QUARTZ, MEASURED AT 700°C. (after Kammer *et al.* 1948)

c_{11}	c_{33}	c_{13}	c_{12}	c_{44}	$c_{66}=\frac{1}{2}(c_{11}-c_{12})$
1.30	1.21	0.44	0.28	0.37	0.51×10^{12} dynes/cm^2

pressure, are invariably of pure screw orientation, or of the particular mixed character given in Table 1.

Another conclusion to be drawn from Table 1 is that a screw dislocation with Burgers vector ***a*** has almost the same non-core energy as a screw dislocation with Burgers vector ***c***, the difference being only 1.5 percent. Consequently, screw dislocations with Burgers vectors ***a*** and ***c*** might be expected to have equal stabilities in high-quartz. This latter conclusion brings out the usefulness of the anisotropic formulae, since isotropic formulae would indicate a difference in energy of 19.2 percent between screw dislocations with Burgers vectors ***a*** and ***c***.

Choice of Slip Systems

Eshelby (1949) defined a measure of the "width" of an edge dislocation as

$$\xi = \tfrac{1}{2} K s'_{66} d \tag{6}$$

where K is the energy factor defined by equation (2), s'_{66} is the compliance (referred to dislocation axes) and d is the interplanar spacing of the glide planes. He further suggested that the ratio ξ/b, where b is the modulus of the Burgers vector, would serve as a measure of the "ease of gliding".

Column 5 in Table 1 lists the calculated dislocation "widths" in terms of the respective Burgers vectors. The values of d and s'_{66} used in the calculations are:

$$(0001)\, d = 1.83 \text{ Å}; \qquad s'_{66} = s_{44} = 26.9 \times 10^{-13} \text{ cm}^2/\text{dyne}$$
$$\{1\bar{1}00\}\, d = 4.44 \text{ Å}; \qquad s'_{66} = s_{66} = 19.4 \times 10^{-13} \text{ cm}^2/\text{dyne}$$
$$\{11\bar{2}0\}\, d = 2.51 \text{ Å}; \qquad s'_{66} = s_{66} = 19.4 \times 10^{-13} \text{ cm}^2/\text{dyne}$$

The d values were calculated from the lattice parameters used earlier, and the s_{ij} (at 700°C) were taken from Kammer *et al.* (1948).

Using Eshelby's criterion for ease of gliding, ξ/b, it is evident from Table 1 (column 5) that the easiest glide system in high-quartz should be $\{1\bar{1}00\} <\bar{1}\bar{1}20>$, followed by the system $\{1\bar{1}00\}$ [0001]. Thus first order prismatic slip in both the directions ***a*** and ***c*** should be preferred over basal slip. This may explain the observation by Griggs and Blacic (1965) that above 700°C, slip is predominantly on prism planes. However, it can be seen that basal slip is preferred over second order prismatic slip $\{11\bar{2}0\}$ [0001].

Structural Considerations

Dislocation theory, based on Frank's energy criterion and the Peierls

stress criterion, predicts that the shorter of the possible perfect-dislocation Burgers vector should correspond to the slip direction, while the glide plane should be the plane with the lowest Peierls stress. In discussing slip in quartz, other structural factors must also be taken into consideration.

Firstly, the slip direction must be such as to avoid strong electrostatic repulsion between like charges. Secondly, the slip direction must also be one which allows the minimum disturbance of the tetrahedrally bonded SiO_4 units, i.e. one which results in the breaking of the least number of bonds.

From the nature of the dislocation cores discussed in paper I, it is evident that dislocations with Burgers vectors $\boldsymbol{a}$ and $\boldsymbol{c}$ satisfy these conditions. Thus the expected slip directions in quartz are parallel to the crystallographic $\boldsymbol{a}$ and $\boldsymbol{c}$ axes. It is also worth noting that as shown above, screw dislocations with either of these two Burgers vectors have equal stabilities in the high-quartz structure.

Considering the slip planes, equation (6) indicates that for a given Burgers vector, the easiest glide plane is the plane with the largest d-spacing, i.e. the least Peierls stress. However, where directional bonding is important, such as in the case of quartz, it is possible that the Peierls stress may be lower for a plane other than that with the largest d-spacing. This possibility was ignored in estimating the "ease of slip" of the various dislocations in the last section, simply because in the original Peierls model used by Eshelby (1949), directional bonding was not considered.

Qualitatively, pairs of SiO_4 units in quartz share corners with each other. Consequently, the glide of dislocations through the lattice inevitably involves the breaking and remaking of some of the tetrahedral Si-O bonds. It is, therefore, intuitively argued that the easiest slip plane is expected to be that across which the Si-O bond density is least.

Table 3 lists the bond densities (measured as the number per unit area within the Unit Cell) across various low index planes containing the lattice vectors $\boldsymbol{a}$, $\boldsymbol{c}$ or $<\boldsymbol{a}+\boldsymbol{c}>$. The "ease of slip" expected on this basis is in the order $\{10\bar{1}1\}$, $\{10\bar{1}0\}$, $\{10\bar{1}2\}$, $\{11\bar{2}0\}$, $\{10\bar{1}3\}$ and (0001), for slip in the directions $\boldsymbol{a}$ or $\boldsymbol{c}$. Thus it is confirmed that first order prismatic slip in either of the directions $\boldsymbol{a}$ or $\boldsymbol{c}$ should be preferred over basal slip in the direction $\boldsymbol{a}$. However, contrary to the theoretical prediction in the last section, second order prismatic slip $\{11\bar{2}0\}$ [0001] appears to be preferred over basal slip (0001) $<\bar{1}\bar{1}20>$.

For slip in pyramidal planes in pyramidal directions $<\boldsymbol{a}+\boldsymbol{c}>$, the "ease of slip" is in the order $\{10\bar{1}1\}$, $\{11\bar{2}2\}$, and $\{11\bar{2}1\}$.

It is apparent from Table 3 that the easiest slip planes in high-quartz are expected to be rhombohedral $\{10\bar{1}1\}$ planes, which have also been

TABLE 3. BOND DENSITIES FOR THE DIFFERENT SLIP SYSTEMS

Slip plane	Slip direction	Si-O bonds per Å^2
$\{10\bar{1}1\}$	$\langle\bar{1}2\bar{1}0\rangle$; $\langle\bar{1}\bar{1}23\rangle$	0.057
$\{10\bar{1}0\}$	$\langle\bar{1}2\bar{1}0\rangle$; [0001]	0.073
$\{10\bar{1}2\}$	$\langle\bar{1}2\bar{1}0\rangle$	0.078
$\{10\bar{1}3\}$	$\langle\bar{1}2\bar{1}0\rangle$	0.085
(0001)	$\langle\bar{1}2\bar{1}0\rangle$	0.092
$\{11\bar{2}0\}$	[0001]	0.084
$\{11\bar{2}1\}$	$\langle1\bar{2}13\rangle$	0.077
$\{11\bar{2}2\}$	$\langle\bar{1}\bar{1}23\rangle$	0.063

predicted to be the planes of easiest cleavage (Niggli, 1926 and Fairbairn, 1939). Experimental evidence of preferred rhombohedral cleavage was reported by Bloss and Gibbs (1963).

Critical Resolved Shear Stress for Slip. Table 4 summarizes the mean resolved shear stress at the yield point (0.2 percent plastic strain) on the

TABLE 4.

Compression axis	Slip system	Critical resolved shear stress in kilobars	
		700°C	800°C
$\perp B$	(0001) $[\bar{1}\bar{1}20]$	0.93	0.78
	$(11\bar{2}0)$ [0001]	0.93	0.78
$\perp a$	$(10\bar{1}0)$ $[\bar{1}2\bar{1}0]$	1.03	0.83
$\perp m$	$(10\bar{1}0)$ $[\bar{1}2\bar{1}0]$	1.06	0.81
$\perp z$	$(10\bar{1}0)$ [0001]	0.97	0.86
	$(\bar{1}102)$ $[\bar{1}\bar{1}20]$	0.97	0.86
	$(1\bar{1}03)$ $[\bar{1}\bar{1}20]$	0.95	0.84
	$(1\bar{1}01)$ $[\bar{1}\bar{1}20]$	0.91	0.81
	$(11\bar{2}0)$ [0001]	0.83	0.72
	(0001) $[\bar{1}\bar{1}20]$	0.83	0.72
$\perp A$	$(\bar{1}011)$ $[\bar{1}2\bar{1}0]$	0.80	0.66
	$(\bar{1}010)$ $[\bar{1}2\bar{1}0]$	0.76	0.62
	$(0\bar{1}12)$ $[2\bar{1}\bar{1}0]$	0.67	0.55
	(0001) $[\bar{1}\bar{1}20]$	0.65	0.54
$\perp C$	$(11\bar{2}2)$ $[\bar{1}\bar{1}23]$		2.31
	$(\bar{1}101)$ $[1\bar{2}13]$		2.12
	$(11\bar{2}1)$ $[\bar{2}113]$		1.43

various slip systems, using a constant strain-rate of 3.1×10^{-5} sec^{-1}. All the slip systems listed were observable at the smallest measurable plastic strains, and in the cases where more than one system of the same type were equally stressed and subsequently observed, only one is given in the table. The orientations of the compression axes are given in paper I.

In specimens compressed $\perp a$ and $\perp m$, the identical values of yield stress serve as a cross-check on the critical resolved shear stress for slip on the systems $\{10\bar{1}0\} <\bar{1}2\bar{1}0>$. However, since for all other orientations of compression different slip systems were observed simultaneously, it was not possible to uniquely assign the critical resolved shear stress for slip on the different systems. The maximum experimental error in the values of stress given in Table 4 is 0.1 kbar, so it is concluded that the critical resolved shear stress for slip in either of the directions $\boldsymbol{a}$ or $\boldsymbol{c}$, and on the low index planes in high-quartz, is more or less the same.

The marginally lower critical resolved shear stress for slip on the rhombohedral $\{10\bar{1}1\} <\bar{1}2\bar{1}0>$ systems is no doubt a reflection of the relatively low Si-O bond density across these planes (Table 3), and of the relative smoothness of the slip surface. (see paper I).

On the other hand, it is evident in Table 4 that the initial resolved shear stress for slip on pyramidal planes and in pyramidal directions is about three times as much as for slip on the slip systems discussed previously. This is attributed to the much larger Burgers vectors of dislocations in these slip systems, since the Peierls stress increases with increasing magnitude of the Burgers vector. It is also of interest to note that slip in directions $<\boldsymbol{a}+\boldsymbol{c}>$ commences only at test temperatures of 750°C and above (see paper I).

DISCUSSION

The two approaches used here to predict the ease of slip in quartz, namely Eshelby's criterion and the bond-densities, both suggest that first order prismatic slip should be easier than basal slip. However, experimental measurements of the critical resolved shear stresses for slip do not reveal the expected difference. Slip appears to have occurred with equal facility on all the low index planes indicated, in either of the directions $\boldsymbol{a}$ or $\boldsymbol{c}$.

Griggs and Blacic (1965) have reported that the mechanism of plastic flow in quartz tested under hydrostatic pressure changes from predominantly basal to predominantly prismatic slip, when the test temperature exceeds 700°C. In the present work conducted at atmospheric pressure, using the slowest strain-rate of 3.1×10^{-5} sec^{-1}, changes in deformation behaviour were also observed with changing test temperature. Thus, bearing in mind the inherent limitations of the two approaches to the

problem of ease of glide used here, and the fact that the development of the different slip systems also depends on other factors such as dislocations intersections etc., the possible preference of prismatic slip over basal slip in high-quartz cannot be ruled out.

It was pointed out in paper I that the SiO_4 tetrahedral units are strongly bonded together and linked to form a three dimensional net, so that the quartz structure is roughly uniformly bonded in three-dimensions. This may be why this structure is denied any planes of easy cleavage. Correspondingly, one would not expect strong crystallographic control of slip, and the factor controlling plasticity could be the ability to nucleate slip dislocations.

The similarities between the nature of the cores of dislocations with Burgers vectors ***a*** or ***c*** discussed in paper I; the equal stabilities of these two types of dislocations in the high-quartz structure shown here, and also, the apparently equal facility of slip in these two directions on various crystallographic planes, all indicate that the important factor in glide deformation in quartz is the slip direction.

Linear elasticity theory cannot be used to estimate the strain energy of the grossly distorted material close to a dislocation line. Should this be a significant part of the total strain energy of a dislocation in quartz, then the structural difference, pointed out in paper I, between the core distortions of dislocations with Burgers vectors having the same magnitude but opposite signs, may also have a strong influence on the glide of dislocations through the lattice.

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References

Baëta, R. D., and K. H. G. Ashbee (1969) Slip systems in quartz I. *Amer. Mineral.*, **53,** 1551–1573.

Bloss, F. D. and G. V. Gibbs (1963) Cleavage in quartz. *Amer. Mineral.* **48,** 821–838.

Christie, J. M., D. T. Griggs, and N. L. Carter (1964). Experimental evidence of basal slip in quartz. *J. Geol.* **72,** 734–756.

Eshelby, J. D. (1949) Edge dislocations in anisotropic materials. *Phil. Mag.* **40,** 903–912.

———, W. T. Read, and W. Shockley (1953) Anisotropic elasticity with applications to dislocation theory. *Acta Met.* **1,** 251–259.

Fairbairn, H. W. (1939) Correlation of quartz deformation with its crystal structure. *Amer. Mineral.* **24,** 351–368.

Foreman, A. J. E. (1955) Dislocation energies in anisotropic crystals. *Acta Met.* **3,** 322–330.

Frondel, C. (1962) *System of Mineralogy of . . . Dana, Vol.* 3. John Wiley and Sons, New York.

Griggs, D. T., and J. D. Blacic (1965) Quartz: anomalous weakness of synthetic crystals. *Science* **147,** 292–295.

KAMMER, E. W., T. E. PARDUE, AND H. F. FRISSEL (1948) A determination of the elastic constants for beta-quartz. *J. Appl. Phys.*, **19**, 265–270.

MCLAREN, A. C., J. A. RETCHFORD, D. T. GRIGGS, AND J. M. CHRISTIE (1967) Transmission electron microscope study of Brazil twins and dislocations experimentally produced in natural quartz. *Phys. Stat. Sol.* **19**, 631–644.

NIGGLI, P. (1962) Beziehungen zwischen Struktur and äußerer Morphologie am Quarz. *Z. Kristallogr.* **63**, 295–311.

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