Experimental Deformation of Quartz Single Crystals

though the main faults in all three types of cylinders are inclined at the same angle (38°) to the axis of compression.

In cylinders compressed perpendicular to m, there is high shear stress on m_2 and m_3 compared with the rhombohedra r_2 , r_3 and z_2 , z_3 , but the main faults are invariably parallel to the rhombohedral planes. Thus faulting appears to take place with greater facility on r and z than m. Similar considerations suggest that shear stresses high enough to cause faulting on the second order prism planes (a) are seldom attained. These conclusions are supported, in a more general way, by the fact that the m and a planes are never present as the main faults, though they are suitably oriented in several types of cylinders.

The evidence clearly indicates that the critical shear stress required for faulting on the basal plane (c) is less than for faulting on the *r* and *z* planes; and the shear stress for faulting on *r* and *z* is considerably less than for the prisms *m* and *a* (table 2).

It is of interest to compare the relative ease of faulting on various crystal planes, as determined above, with the ease of cleavability on these planes. Shappell (1936) and Fairbairn (1939) have calculated the ease of cleavability of quartz parallel to planes of low indices, using the criterion that cleavage will tend to occur along planes that cut the minimum number of bonds per unit area; Fairbairn considered the α -quartz structure and Shappell that of β quartz. In decreasing tendency to cleave, Shappell lists the planes in the order r and z, a, c, m; Fairbairn lists them in the order r and z, m, c, a. Observations of natural cleavage in quartz (Fairbairn, 1939) support these inferences in that the commonest and most perfect cleavages are invariably parallel to the unit rhombohedra. Cleavage fractures are essentially extension fractures, and both investigators, in deriving their results, considered a tensile stress acting normal to the planes. The density of bonds in the planes might also be expected to influence fracture in response to shear stress on the planes, but it is evident that such considerations do not predict the ease of faulting on these planes, since the shear stress necessary to produce faulting on the base (c) is less than that for faulting on r and z.

It is possible to estimate the theoretical shear strength ("molecular cohesion") of crystals from considerations of the stress required to move an atom in any row into the next similar site in the lattice (Cottrell, 1953). According to the original calculation and assumptions of Frenkel, the critical shear stress necessary to produce such a displacement in a perfect crystal ($\tau_{\rm m}$) should be $\tau_{\rm m} = \frac{\rm b}{\rm a} \cdot \frac{\mu}{2\pi}$, where a is the spacing between the planes along which displacements occur, b is the distance between similar atomic sites in the direction of displacement, and μ is the shear modulus in the direction of displacement. Since a b in most crystals $\tau_{\rm m} \cong \frac{\mu}{2\pi}$. Subsequent refinements of this calculation indicate that the theoretical shear strength of most crystals may be as low as $\frac{\mu}{30}$ (Cottrell, 1953, p. 9).

In the majority of crystalline materials plastic deformation occurs at stresses several orders of magnitude lower than the theoretical strength, but it

47

J. M. Christie, H. C. Heard, and P. N. LaMori

is well known that quartz and other brittle materials, deformed in compression, may support stresses much closer to the theoretical strength before rupture or plastic flow occurs. The shear moduli in quartz are a few hundred kilobars, and the theoretical shear strengths are therefore an order of magnitude less than this. In compression experiments on quartz at room temperature and pressure, the maximum shear stress in the samples at rupture is approximately 10 kb. At the high confining pressure of the present series of experiments, the shear stress on the main faults at rupture is over 20 kb. The measured shear stresses are therefore within the range of the estimated theoretical values. In view of this, it is of interest to determine whether the shear stress necessary to produce faulting on the various planes varies in the same way as the shear moduli or the theoretical strengths for these planes, calculated according to the above equations.

The shear moduli for certain directions in the planes c, r, z, m, and a are given in table 3. The values in the table are components C_{ijij} of the elastic stiffness tensor $[C_{ijkl}]$, relating the shear stress (σ_{ij}) in the direction of increasing X_i on the plane perpendicular to the coordinate axis X_j , to the shear strain in the same direction on the same plane (ε_{ij}) . The elastic stiffness constants (C_{ijkl}) were calculated from values of the compliance constants (S_{ijkl}) given by Nye (1957, p. 148). The moduli in the required directions were determined by transformation (in cases where this was necessary) according to the standard law for a fourth-rank tensor: $C_{ijij} = a_{im}a_{jn}a_{io}a_{jp}C_{mnop}$. The transformations were carried out with a Bendix G15 computer.

The significance of these values for the problem under consideration is open to doubt, for the following reasons: (1) The elastic constants used in the calculations were determined at low pressure, and the behavior may not be linear up to the high pressures in the experiments; (2) the simple model from which the expression for theoretical strength is derived is a reasonable one for metal structures, but its relevance for a complex framework structure like that of quartz is doubtful. It is clear, in any case, that the relative ease of faulting on the planes c, r, z, m, and a is not related either to the shear moduli or the theoretical strengths, as calculated above.

Plane	Direction	Shear modulus Cıjıj (kb)	b a	$\frac{C_{ijij}}{2\pi}$	$\left(\frac{b}{a},\frac{C_{ijij}}{2\pi}\right)$	C1111 30
c {0001}	$<01^{\dagger}0>(\perp m)$ $<10^{\dagger}0>(a)$	571 571	1.58 0.91	90.9 90.9	143.6 82.7	19.0 19.0
r {10I1}	<10†1>	384	4.07	61.1	248.7	12.8
z {01I1}	<01†1>	461	4.07	73.4	298.7	15.4
m {10I0}	[0001] <10†0>	571 398	1.29 1.15	90.9 63.4	117.3 72.9	19.0 13.3
a {1120}	[0001] <01†0>	571 398	$2.20 \\ 3.47$	90.9 63.4	200.0 220.0	19.0 13.3

TABLE 3

Shear moduli and theoretical strengths for various planes and directions