

## Observation of Crystal Plasticity under High Pressure with Applications to the Earth's Mantle

ROBERT B. GORDON

*Department of Geology and Geophysics, Yale University,  
New Haven, Connecticut 06520*

Direct experimental measurement shows the activation volume for the motion of glide dislocations in crystals always to be less than the activation volume for thermally activated atom movements. The activation volumes for thermally activated atom movements remains, therefore, the rate limiting step in plastic flow at all depths in a mantle composed of solid close-packed oxides. The occurrence of partial melting and of pressure-induced phase transformations is expected to result in zones of low shear strength in the mantle. Plastic flow may largely be localized to these zones.

The motions thought to be occurring in the earth's mantle require rock to flow by plastic deformation. A test that can be applied to theories of these motions is that they be consistent with what can be inferred from solid-state physics about the plastic properties of rock under the temperature, pressure, and stress existing in the mantle. There is extensive experimental and theoretical knowledge of the plastic properties of crystalline materials at high temperature, but not of the response of solids to small deviator stresses in the presence of a large hydrostatic stress component, the stress state in the mantle. Many experiments on crystal plasticity have been made with samples placed under high pressure to suppress brittle fracture; the pressure dependence of the plastic flow properties has not been observed. In this paper the results of a series of experiments that establishes the pressure sensitivity of basic mechanisms of crystal slip are summarized and applied to the problem of the plastic properties of the earth's mantle.

Experiments in which plastic properties are observed under conditions duplicating the physical and chemical environment of the upper mantle are not yet possible. Instead, inferences about plastic properties must be drawn from knowledge of the basic deformation mechanisms active in all solids. Small-scale deformation at a slow rate can be achieved without dislocation motion by individual atom movements

alone (Nabarro-Herring creep). Large-scale deformation of a crystalline material is accomplished by the motion of glide dislocations. Barriers to the motions of dislocations can be removed or circumvented by thermally activated atom movements at high temperature. Steady-state creep results when the stress is low and the temperature high; then, at room pressure atomic mobility is rate limiting for this type of creep.

The variation of crystal plasticity with depth in a homogeneous mantle is dependent on how both atomic mobility and dislocation mobility change with pressure and temperature. The pressure and temperature dependence of the rate of atom movement is given by

$$\tau = \tau_0 e^{G^*/kT} \quad (1)$$

where  $\tau$  is the mean residence time of an atom on a lattice site and the activation free energy  $G^* = E^* + PV^* - TS^*$  depends on the activation energy  $E^*$ , volume  $V^*$ , and entropy  $S^*$ . In close-packed oxide structures  $V^*$  is about equal to the oxygen atomic volume  $V_o$ . Equation 1 can be used to estimate the dependence of atomic mobility in close-packed oxide crystals on depth in the earth [Gordon, 1965].

The motion of glide dislocations in a crystal can also be described in terms of rate theory since dislocation movements are thermally activated. The strain rate resulting from slip on a particular glide system is [Gilman, 1965]

$$\dot{\epsilon}' = \phi b N v = \phi b (N_0 + M \epsilon) v_0 e^{-(D+W\epsilon)/\sigma} \quad (2)$$

In this equation  $\phi$  is a factor that allows for the orientation of the active slip system,  $b$  is the Burgers vector,  $N$  is the dislocation density, and  $v$  is the mean dislocation velocity. The second form of the equation is found experimentally to represent well the plastic deformation curves for many crystals. The coefficient  $M$  measures the rate at which dislocations multiply as deformation proceeds,  $D$  is a measure of dislocation mobility in the undeformed crystal, and  $W$  allows for work hardening. Because dislocations overcome obstacles on the glide plane with the aid of thermal energy

$$v = v_0 e^{-(D+W\epsilon)/\sigma} = e^{-G^*/kT} \quad (3)$$

showing that the activation free energy  $G^*$  is stress dependent for dislocation motion.

Consider now how the strain rate is altered on application of hydrostatic pressure. The term  $N_0 + M\epsilon$  in equation 2 is hardly changed even at the pressures of the earth's deep interior. The term remains almost unchanged because the formation energy of a dislocation  $E_f$  is large and the volume of formation  $V_f$  is small, so that  $PV_f \ll E_f$ . The influence of pressure on strain rate is through the velocity term in equation 2. The thermodynamic quantity describing this dependence is  $V_a^*$ , whose definition is seen from equation 4 [Li, 1967]

$$\begin{aligned} d \ln v &= \left( \frac{\partial \ln v}{\partial \sigma} \right)_{T, P, \epsilon} d\sigma + \left( \frac{\partial \ln v}{\partial T} \right)_{P, \sigma, \epsilon} dT \\ &+ \left( \frac{\partial \ln v}{\partial P} \right)_{\sigma, \epsilon, T} dP + \left( \frac{\partial \ln v}{\partial \epsilon} \right)_{\sigma, P, T} d\epsilon \\ &= \frac{D + W\epsilon}{\sigma^2} d\sigma + \frac{H^*}{kT^2} dT - \frac{V^*}{kT} dP - \frac{W}{\sigma} d\epsilon \end{aligned} \quad (4)$$

to be

$$V^* = kT \left( \frac{\partial \ln v}{\partial P} \right)_{\sigma, \epsilon, T} \quad (5)$$

Equation 5 specifies that  $V_a^*$  is to be measured by finding the change in dislocation velocity with pressure in an experiment done at constant stress, strain, and temperature. Observations of this kind can be made in experiments in which the motion of individual dislocations is observed directly, as is done, for example, when dislocation intersections with a free sur-

face are identified by etch pits. The crystal to be studied is subjected to a given deforming stress for a given time with and without hydrostatic confining pressure applied. The average displacements of mobile dislocations are observed by successive etching and from these data the average dislocation velocities are calculated. Since the total dislocation displacement remains small,  $\epsilon$  is effectively constant during the experiment.

A set of direct dislocation velocity measurements is shown in Figure 1. The scatter in the data is such that  $\partial \ln v / \partial P$  is not detected. The scatter arises because dislocations do not advance under a given shear stress at a uniform velocity. They move instead by a series of jumps (in which  $v$  is nearly the sound wave velocity) separated by periods of rest. Successive jumps are

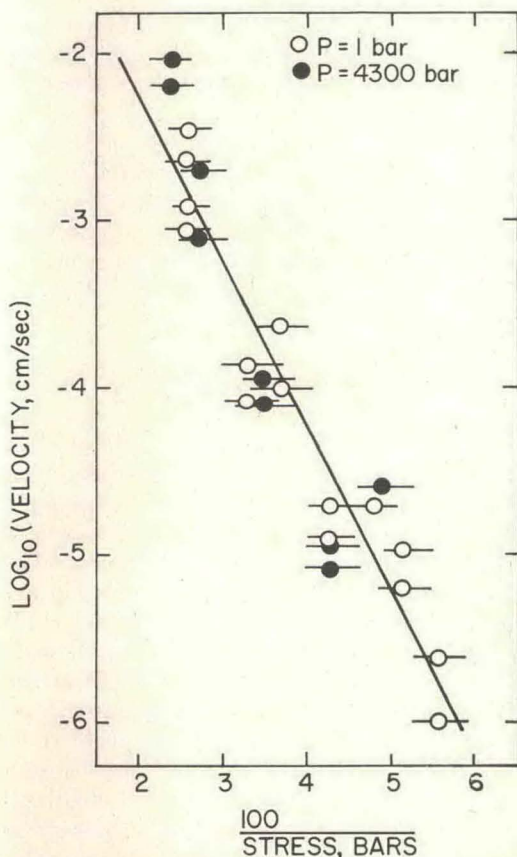


Fig. 1. Results of direct measurements of the velocity of screw dislocations in LiF single crystals with and without applied hydrostatic pressure [Haworth, 1969].

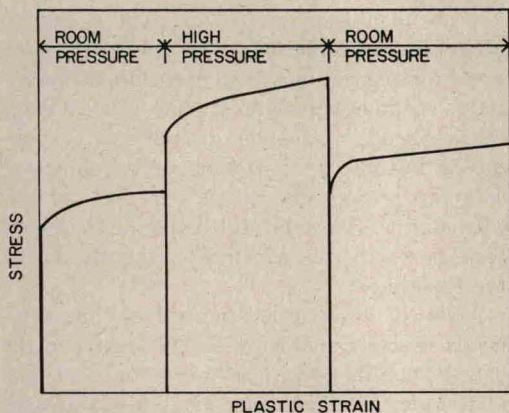


Fig. 2. Method of finding the pressure dependence of the plastic flow stress of a crystal by mechanical testing.

thermally activated and occur at random. The number of displacements that must be averaged to get a reliable mean velocity is so large that the method of direct observation is impractical for determination of  $\partial \ln v / \partial P$ .

When the strain resulting from plastic glide on a particular slip system is observed, the result of the motion of many individual dislocations is automatically averaged. The activation volume for dislocation movement in a macroscopic stress-strain experiment can then be found from

$$V^* = kT \left( \frac{\partial \ln \dot{\epsilon}'}{\partial \ln \sigma} \right)_{T,P,N} \left( \frac{\partial \ln \sigma}{\partial P} \right)_{T,v,N} \quad (6)$$

The first derivative represents a room pressure determination of the strain rate sensitivity of the plastic flow stress. The second is measured by the increment in stress required to keep a crystal deforming at constant dislocation velocity when hydrostatic pressure is suddenly applied. The appropriate experimental method for determining this value is illustrated in Figure 2. The deforming stress and plastic strain are measured while the crystal is subjected to repeated small deformations. When there is no change in environmental conditions between successive deformations (and there are no large recovery effects), nearly continuous stress-strain curve is generated. When hydrostatic pressure is applied during some of the deformations, a different stress is required to continue the plastic flow (as shown in Figure 2); release of the pres-

sure results in a reversal of the incremental stress.

That a good approximation to the idealized experiment described above can be achieved in practice is shown by the data displayed in Figure 3 for the deformation in compression of a single crystal of CsBr [Davis and Gordon, 1968]. Successive applications of stress at constant pressure generate a smooth  $\sigma$ - $\epsilon$  curve and the application of hydrostatic pressure results in a reversible increment in flow stress. The conditions that  $v$  and  $N$  be constant are met because the stress increment  $\delta\sigma$  is measured at a given strain and because the experiment is done in such a way that the rate of plastic deformation is the same at both pressures.

Experiments of the type illustrated in Figure 3 have been performed on a wide variety of crystalline materials (unpublished data obtained by E. Aladag, W. L. Haworth, and L. A. Davis, 1970). The results obtained on metals, alloys, and covalently bonded compounds (selenides) can be summarized as follows. In these materials the fractional increment of plastic flow stress  $\delta\sigma/\sigma$  is always less than or equal to the fractional increment of the shear modulus  $\delta\mu/\mu$  that results from the application of hydrostatic pressure. (The shear modulus to be used is the elastic coefficient for the type of dislocation under study.) This means that  $V_a^* \ll V_a$ , that dislocation motion is very much less pressure sensitive than thermally activated atom movements. The active deformation mechanism is such that the strength of the above materials arises from the elastic interactions between dislocations, or between dislocations and point de-

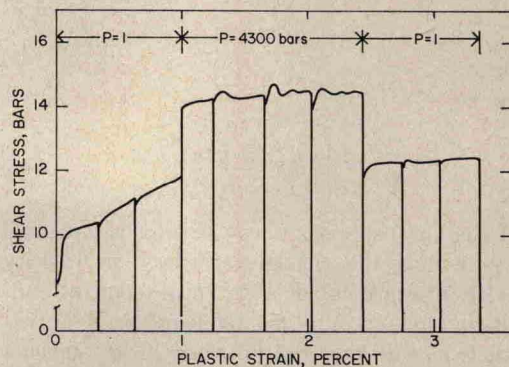


Fig. 3. Compression tests on a single crystal of CsBr with and without applied hydrostatic pressure [Davis and Gordon, 1968].

fects or solute atoms. Under pressure the deformation mechanism does not change and the strength is increased by as much as the shear modulus, and, hence, the interaction force, is increased.

In ionic crystals a wider variety of phenomena appear [Davis and Gordon, 1968]. The strength may again be controlled by elastic interactions (as in irradiated crystals) in which case the response to pressure is like that of the other classes of materials. However, in the initial stages of deformation of very pure alkali halides, large increments in flow stress are found;  $V_a^* \simeq V_a$ . The rate limiting step in the deformation of these materials is the generation of vacancies by moving dislocations; hence, the large activation volume results. During deformation of these materials  $V_a^*$  decreases because the elastic interaction between dislocations generated during the plastic flow soon dominates the deformation process (work hardening). In the ionic crystals NaCl and KCl it is found that after heavy deformation (into the third stage of work hardening) application of hydrostatic pressure results in a decrease in flow stress and a decrease in work hardening rate [Davis and Gordon, 1969]. A detailed explanation of this phenomenon can be given. Glide occurs on the dodecahedral system  $\{110\}\langle 110 \rangle$ . The glide dislocations are dissociated into pairs of partial dislocations separated by a stacking fault. In this fault ions of like sign are brought closer together than in the normal crystal structure and there results a dilatation of the crystal. Application of hydrostatic pressure increases the energy of formation of the stacking fault so that the partial dislocations move closer together. This facilitates the recombination of the partials required for cross slip, the rate limiting step in the third stage of deformation. The model is confirmed by quantitative calculations [Haasen *et al.*, 1970].

The results of the experiments on single crystals can be summarized by saying that, although a variety of different deformation mechanisms, each with a characteristic activation volume, have been observed, in none of these mechanisms is the activation volume greater than that for thermally activated atom movements. Although the data now available are not so extensive, it appears that the same statement can be made for polycrystals. Defor-

mation of a polycrystal, particularly in a material of low symmetry, requires the action of more slip systems than are ordinarily observed in experiments on single crystals. Often the glide characteristics on the secondary systems have a very different temperature and strain rate sensitivity than the primary system has, and, since glide on the secondary systems is usually rate limiting in polycrystals, the polycrystal may have mechanical characteristics quite different from those of single crystals of the same material. In the alkali halides, for example, the yield stress for the cube glide,  $\{100\}\langle 110 \rangle$  has a much greater temperature coefficient than yield stress for dodecahedral glide  $\{110\}\langle 110 \rangle$ . The same is not true for the pressure sensitivity. Experiments in which NaCl and KCl crystals are deformed in torsion (so that glide is confined to the secondary cube system) show a smaller  $V_a^*$  than is obtained for the primary glide system (L. A. Davis and R. B. Gordon, unpublished data, 1970). The pressure dependence of the plasticity of the polycrystal is expected, then, to be similar to that of the single crystals, as has been confirmed for NaCl: Polycrystals deformed under high pressure have a lower plastic flow stress than polycrystals deformed at room pressure (Figure 4) [Aladag *et al.*, 1970].

#### APPLICATION TO THE MANTLE

The ratio  $T/T_m$  of local temperature to the melting temperature is important in determining the type of plastic flow occurring in the mantle. This ratio varies with depth as shown in Figure 5. Throughout the mantle it is greater than 0.5, whereas in the upper mantle it is near (or possibly above) unity. Consequently hot creep is expected to be the dominant mode of deformation in an all-solid mantle composed of close-packed oxides. Since the experiments show that  $V_a^* < V_a$  for all hardening mechanisms, it follows that thermally activated atom movements will remain the rate limiting step in hot creep at all depths. The depth dependence of the effective viscosity for hot creep will then be generally the same as the depth dependence of the viscosity in diffusion creep. Curves of effective viscosity versus depth in the mantle have been developed on this basis by Weertman [1970]; the general form is that shown in Figure 6.

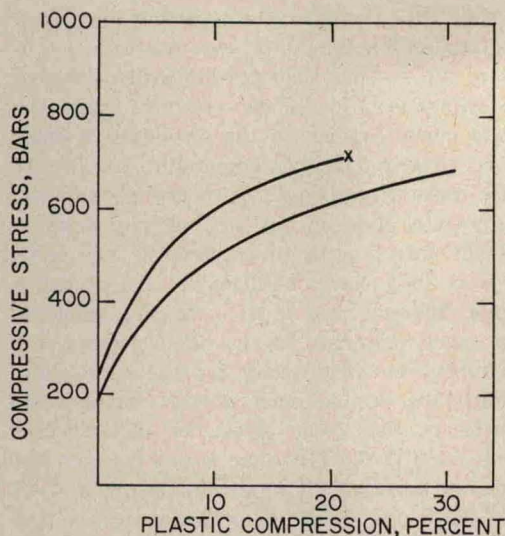


Fig. 4. Plastic compression curve for NaCl polycrystals at room pressure and at high pressure [Aladag *et al.*, 1970]. Lower curve is for  $T = 4$  kb.

The experimental results for polycrystalline NaCl show a softening due to the application of high pressure. Could a similar effect occur at any place in the mantle? In order for this to occur it would be necessary for the rate limiting step in the deformation to be controlled by slip on a glide system where dislocations dissociate to produce a stacking fault with unlike ions brought closer together than they are in the normal crystal. Such dislocations have not been found in any of the minerals likely to be im-

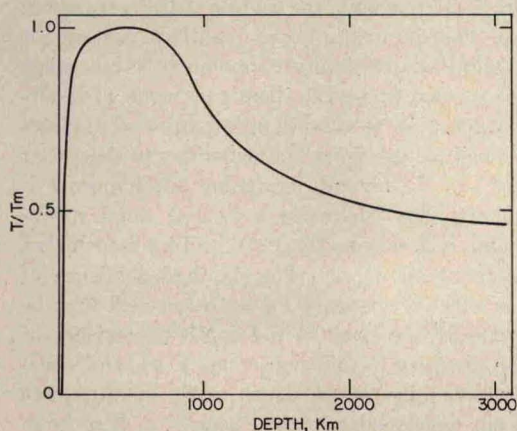


Fig. 5. The ratio  $T/T_m$  versus depth in the mantle.

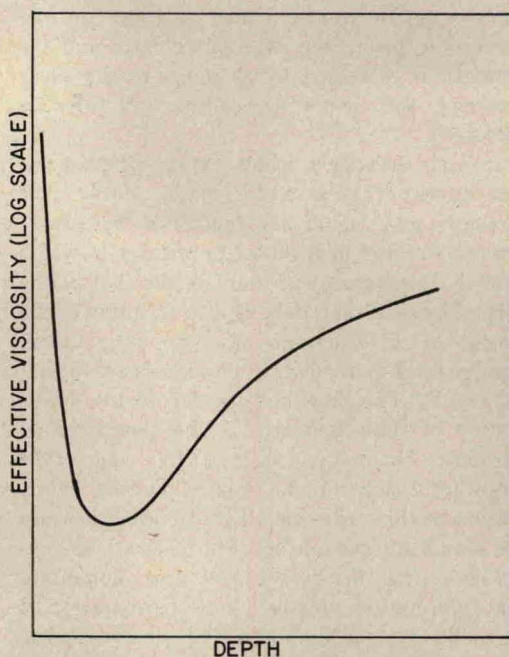


Fig. 6. The general form of the variation of effective viscosity with depth in the mantle.

portant mantle constituents, but their occurrence is theoretically possible. However, pressure softening is expected to occur only when  $T/T_m \leq 0.5$ . At higher temperatures recombination of partial dislocations is no longer the rate limiting step. Consequently pressure softening is unlikely to be important in the mantle.

The above observations apply for a mantle composed of dense polycrystalline oxide. Two processes, which are likely to occur in the mantle, could alter them significantly. These are partial melting and pressure-induced phase transformations. Small amounts of melt formed at grain boundaries are not expected to alter the rate of hot creep. Plastic deformation of individual grains must still occur, and it remains the rate limiting step. Because of the melt stresses are relaxed at the grain boundaries, but they would be relaxed in any case because of the relatively low viscosity of a solid grain boundary at high temperature (revealed, for example, by the grain boundary internal friction [Gordon and Nelson, 1966]). A change in gross mechanical properties will occur when the volume fraction of melt becomes large enough for mass transport through the melt to become

the dominant source of change of grain shape. The conditions for this to occur and the constitutive relation that will result have yet to be found. It is expected however that such a liquid-solid system will display Newtonian viscosity.

Seismic velocity data in the mantle indicate phase changes to denser oxide structures occurring at certain critical depths. It is expected that plastic properties will be altered in the zone of transition between two phases. Such an effect has been observed in steel. When the transformation of austenite to either martensite or pearlite occurs under an applied deviator stress, extensive plastic deformation accompanies the phase change [Porter and Rosenthal, 1959]. A similar effect has recently been observed during the pressure-induced transformation of RbI from the fcc to the sc crystal structure (Davis and Gordon, unpublished data, 1970). This transformation involves a 13.5% reduction in volume and occurs at 3.5 kb [Pistorius, 1965]. When hydrostatic pressure is applied to a single crystal of RbI, its strength increases in the usual way at all pressures up to the transition pressure. Single-crystal experiments cannot be made on the high-pressure phase because the transformation to the dense phase always converts the single crystal to a polycrystal.

Observations of the strength properties during transformation can be made on polycrystalline samples. An experimental complication that must be overcome is the separation of dimensional changes due to the volume change on transformation from the dimensional changes due to plastic deformation. An experiment in which this separation is accomplished uses the test procedure illustrated in Figure 7. The sample is placed between the platens of a compression test machine and is transformed to the dense phase at a pressure well above 3.5 kb. Pressure is slowly lowered while the platens of the testing machine are separated in such a way that no compressive load develops on the sample owing to its volumetric expansion. When the transformation to the less dense phase commences (at a pressure near 3.5 kb, there is some hysteresis in the transformation pressure), the platens are clamped. One dimension of the sample must then remain fixed. The force necessary to maintain the fixed platens is measured. As the crystal transforms, its volume increases

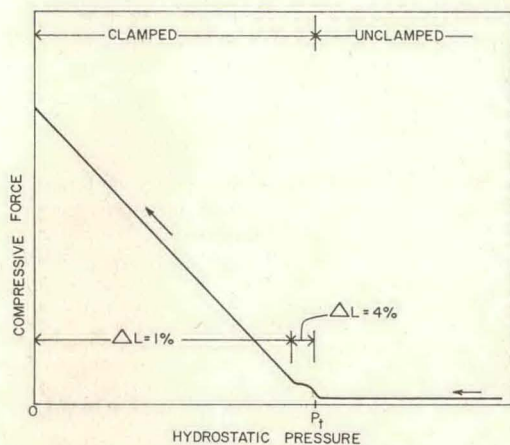


Fig. 7. Compressive loading experiment on a RbI polycrystal.

by 13.5%; it is therefore plastically deformed by an amount equivalent to compression of 4%. The clamping force increases by only a small amount. After transformation is completed, the pressure is reduced to zero and the fcc phase expands a further 1%. The required clamping force now increases by a much larger amount; this additional increase shows that the crystal is substantially weaker while the transformation is in progress than it is after completion of the transformation. From these data it is estimated that compressive strength is reduced by a factor of 7 during the transformation.

This reduction in strength is due to the removal of barriers to dislocation motion by the passage through the grains of interfaces between the two phases. In this sense the transformation is similar to recrystallization. Hence the reduction in strength will occur even when the crystal is being deformed in creep at  $T/T_m > 0.5$ . In the zones of the mantle where a high-pressure and a low-pressure phase coexist, the material present will be relatively weakened as long as the transformation between the phases continues. Continued transformation could result, for example, from the upward passage of deep mantle material through the transformation zones.

The occurrence of partial melting and of pressure-induced phase transformation in the mantle can result in zones in which the yield strength is substantially lowered as compared with the surrounding material. It is reasonable

to expect strong inhomogeneities in the strength properties of the mantle and to suppose that the flow processes responsible for the observed motions are largely localized to these zones of low strength.

*Acknowledgment.* The research results reported have been obtained with financial support from the U. S. Office of Naval Research, Washington, D.C., and the Army Research Office, Durham, North Carolina.

## REFERENCES

- Aladag, E., L. A. Davis, and R. B. Gordon, Cross slip and the plastic deformation of NaCl single and polycrystals at high pressure, *Phil. Mag.*, *21*, 469-478, 1970.
- Davis, L. A., and R. B. Gordon, Pressure dependence of the plastic flow stress of alkali halide single crystals, *J. Appl. Phys.*, *39*, 3885-3897, 1968.
- Davis, L. A., and R. B. Gordon, Plastic deformation of alkali halide crystals at high pressure: Work hardening effects, *J. Appl. Phys.*, *40*, 4507-4513, 1969.
- Gilman, J. J., Microdynamics of plastic flow at constant stress, *J. Appl. Phys.* *36*, 2772-2777, 1965.
- Gordon, R. B., Diffusion creep in the earth's mantle, *J. Geophys. Res.*, *70*, 2413-2418, 1965.
- Gordon, R. B., and C. W. Nelson, Anelastic properties of the earth, *Rev. Geophys.*, *4*, 457-474, 1966.
- Haasen, P., L. A. Davis, E. Aladag, and R. B. Gordon, On the mechanism of stage III deformation in NaCl single crystals, *Ser. Met.*, *4*, 55-56, 1970.
- Haworth, W. L., The effect of pressure on dislocation mobility in ionic crystals, Ph.D. thesis, Yale University, New Haven, Connecticut, 1969.
- Li, J. C. M., Dislocation dynamics in deformation and recovery, *Can. J. Phys.*, *45*, 493-508, 1967.
- Pistorius, C. W. F. T., Polymorphic transitions of the alkali bromides and iodides at high pressures to 200°C, *J. Phys. Chem. Solids*, *26*, 1003-1011, 1965.
- Porter, L. F., and P. C. Rosenthal, Effects of applied tensile stress on phase transformations in steel, *Acta Met.*, *7*, 504-514, 1959.
- Weertman, J., The creep strength of the earth's mantle, *Rev. Geophys. Space Phys.*, *8*, 145-168, 1970.

(Received September 9, 1970.)