

## Brief Report

## Elastic Properties of Polycrystalline Periclase

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New data on the variation with pressure of the elastic parameters of a hot-pressed specimen of MgO are reported. Within the uncertainty of the measurements the elastic constants are independent of direction but the pressure derivatives are not.

The elastic parameters of periclase (stoichiometric MgO) are important for several reasons. Because flawless centimeter-sized single crystals, both natural and synthetic, are available, data of very high precision can be obtained with the usual ultrasonic techniques. Polycrystalline aggregates that have been hot-pressed to nearly theoretical density yield equally precise data. Such data can be used to model the behavior of ionic materials, to test the forms of equations of state, to test the validity of both the Voigt-Reuss-Hill approximation and the improved limits of the Hashin-Shtrikman bounds, and so on. Of equal importance in geophysics is the consideration that periclase is a rock-forming mineral and may be present in the mantle as a separate phase.

The recent publication by Schreiber and Anderson [1968] of a new set of elastic data on polycrystalline MgO that differ considerably from their earlier data [Anderson and Schreiber, 1965] prompts us to publish additional data obtained on another hot-pressed specimen.

The elastic properties of a hot-pressed cube of polycrystalline periclase, cut from one of the eight specimens used in an earlier study of elastic constants at room temperature of this material [Chung, 1963], were measured as a function of hydrostatic pressure to about 10 kb with the McSkimin pulse-superposition method. The microstructural characteristics of this specimen were described in detail in Chung [1963]. The chemical purity was 99.7% MgO. The specimen density was 3.582 g/cm<sup>3</sup> at 25°C. The

experimental procedure followed in the present work was described previously [Chung and Simmons, 1968].

The primary data measured in our ultrasonic experiments were (1) *P* and *S* velocities in three mutually perpendicular directions of the specimen at 25°C, and (2) pulse-repetition frequencies corresponding to these velocities as a function of hydrostatic pressure to 10 kb. The frequencies were linear with pressure. The first pressure derivatives of isotropic elastic moduli were then found from

$$\left(\frac{dM_i}{dP}\right)_{P=0} = \left(\frac{M_i}{3K_T}\right)_{P=0} + \left[M_i \cdot \frac{d}{dP} \left(\frac{F_{iP}}{F_{i0}}\right)^2\right]_{P=0} \quad (1)$$

where  $F_{i0}$  and  $F_{iP}$  are the corrected pulse-repetition frequencies at zero pressure and at pressure *P*, respectively.  $K_T$  is the isothermal bulk modulus (i.e.,  $K_T = K_s/(1 + \alpha T \gamma)$ , where the quantity  $(1 + \alpha T \gamma)$  is 1.0147 at 25°C) and  $M_i$  is an elastic modulus. The subscript *j* refers to either longitudinal or shear modulus. From the values of  $\{dM_j/dP\}_{P=0}$  we calculated values of the first pressure derivatives of velocities from

$$\left\{\left(\frac{\partial V_i}{\partial P}\right)_T\right\}_{P=0} = \left\{\frac{1}{2\rho_0 V_i} \cdot \left[\left(\frac{\partial M_i}{\partial P}\right)_T - \frac{\rho_0(1 + \alpha T \gamma)(V_i)^2}{K_s}\right]\right\}_{P=0} \quad (2)$$

where  $\rho_0$  is the initial density of the specimen.



TABLE 1. Experimental Elastic Data for Polycrystalline Periclase  
 $\rho_0 = 3.582 \text{ g/cm}^3$ , at  $25^\circ\text{C}$ .

| Elastic Properties*                              | Specimen Directions† |        |        | Recommended Values<br>(Arithmetic Mean) |
|--|----------------------|--------|--------|---|
|  | I                    | II     | III    |   |
| $V_p$ , km/sec                                   | 9.717                | 9.690  | 9.687  | 9.698                                   |
| $V_s$ , km/sec                                   | 6.028                | 6.004  | 5.995  | 6.009                                   |
| $\rho_0 V_p^2$ , $10^{11}$ dynes/cm <sup>2</sup> | 33.821               | 33.634 | 33.613 | 33.689                                  |
| $\rho_0 V_s^2$ , $10^{11}$ dynes/cm <sup>2</sup> | 13.016               | 12.912 | 12.874 | 12.934                                  |
| $K_s$ , $10^{11}$ dynes/cm <sup>2</sup>          | 16.467               | 16.418 | 16.448 | 16.444                                  |
| $V_p'$ , $10^{-3}$ (km/sec)/kb                   | 8.10                 | 7.71   | 7.58   | 7.80                                    |
| $V_s'$ , $10^{-3}$ (km/sec)/kb                   | 3.93                 | 3.72   | 3.60   | 3.75                                    |
| $(\rho V_p^2)'$                                  | 7.72                 | 7.43   | 7.34   | 7.50                                    |
| $(\rho V_s^2)'$                                  | 2.50                 | 2.40   | 2.34   | 2.41                                    |
| $K_s'$   | 4.39                 | 4.23   | 4.22   | 4.28                                    |

\* Primes denote the isothermal derivative with respect to pressure.

† Three directions are orthogonal; direction I is parallel to the pressing direction.

In Table 1 the results of these calculations along with the measured quantities are summarized. Direction I is parallel to the direction of hot-pressing.

It should be noted that for the three orthogonal directions the largest differences in  $P$  and  $S$  velocities at room conditions were 0.3 and 0.5% of the mean values. These differences are about the same size as the estimated measurement errors; at room conditions, therefore, this

specimen was considered *elastically isotropic*. Note that  $dV_p/dP$  and  $dV_s/dP$  depend on direction, and each shows about 8% difference. Because these differences are more than twice the size of the estimated experimental errors, we infer that the specimen is anisotropic with respect to the velocity derivatives. Pressure derivatives of elastic properties measured in one direction only of a hot-pressed specimen may not yield correct isotropic values of the aggregate

 TABLE 2. Comparison of Elastic Data from Several Sources  
 All data are at  $25^\circ\text{C}$ .

| Properties*                              | Chung [1963]         | Anderson<br>and<br>Schreiber | Soga and<br>Anderson | Chung and<br>Buessem [1967]† | Schreiber<br>and<br>Anderson | Present Work          |
|--|----------------------|------------------------------|----------------------|------------------------------|------------------------------|-----------------------|
|  |                      | [1965]                       | [1966]               |                              | [1968]                       |                       |
| $\rho_0$ , g/cm <sup>3</sup>             | 3.581                | 3.5800                       | 3.581                | 3.5819                       | 3.5797                       | 3.582                 |
| $V_p$ , km/sec                           | 9.68 ( $\pm 0.06$ )  | 9.7662                       | 9.723                | 9.693 ( $\pm 0.025$ )        | 9.6605                       | 9.698 ( $\pm 0.020$ ) |
| $V_s$ , km/sec                           | 6.00 ( $\pm 0.03$ )  | 5.9635                       | 6.039                | 6.008 ( $\pm 0.012$ )        | 5.9974                       | 6.009 ( $\pm 0.010$ ) |
| $V_p'$ , $10^{-3}$ (km/sec)/kb           |                      | 7.71                         |                      |                              | 8.66                         | 7.80 ( $\pm 0.11$ )   |
| $V_s'$ , $10^{-3}$ (km/sec)/kb           |                      | 4.35                         |                      |                              | 4.23                         | 3.75 ( $\pm 0.08$ )   |
| $K_s'$                                   |                      | 3.916                        |                      |                              | 4.58                         | 4.28                  |
| $\sigma'$ , $10^{-5}$ (kb) <sup>-1</sup> |                      | 5.63                         |                      |                              | 19.5                         | 18.4                  |
| $\sigma$                                 | 0.18                 | 0.203                        | 0.186                | 0.187                        | 0.186                        | 0.187                 |
| $\mu$ , $10^{11}$ dynes/cm <sup>2</sup>  | 12.90 ( $\pm 0.10$ ) | 12.73                        | 13.06                | 12.93                        | 12.88                        | 12.934                |
| $K_p$ , $10^{11}$ dynes/cm <sup>2</sup>  | 16.0                 | 17.17                        | 16.44                | 16.41                        | 16.24                        | 16.444                |
| $K_T$ , $10^{11}$ dynes/cm <sup>2</sup>  |                      | 16.91                        |                      |                              |                              | 16.206                |
| $K_T'$                                   |                      | 3.94                         |                      |                              |                              | 4.35†                 |

\* Primes denote isothermal pressure derivatives.

† Based on Chung's [1966] measurements but taken an arithmetic mean of three values determined on the three orthogonal directions of the specimen.

‡ Calculated from  $B^s$  by using Overton's [1962] equation.



gate. We believe the mean value is likely to be near the correct value for this aggregate.

The present data are compared in Table 2 with some recent data from the literature. For the pressure derivatives of isotropic elastic parameters, our data differ significantly from the corresponding values reported by *Anderson and Schreiber* [1965] and by *Schreiber and Anderson* [1968]. Apparently, Anderson and Schreiber measured the properties of their hot-pressed specimens in one direction only. Yet a typical hot-pressed aggregate of polycrystalline periclase often exhibits preferred orientation of the crystal grains [see, for example, *Tagai et al.*, 1967] with obvious effects on the elastic properties. We suggest that the apparent differences among the several sets of data reported by Anderson and Schreiber and by us here are possibly attributable to this preferred orientation produced by hot-pressing. Of course, the elastic properties may vary from sample to sample, but the important point of this paper is that, at least in certain respects, hot-pressed aggregates may be anisotropic and measurements on such samples should be made in more than one direction.

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## REFERENCES

- Anderson, O. L., and E. Schreiber, The pressure derivatives of the sound velocities of polycrystalline magnesia, *J. Geophys. Res.*, **70**, 5241, 1965.
- Chung, D. H., Elastic moduli of single-crystal and polycrystalline MgO, *Phil. Mag.*, **8**(89), 833, 1963. (See Table 3 on page 840.)
- Chung, D. H., Elastic anisotropy of single-crystals and the polycrystalline isotropic elastic moduli of solids, Ph.D. thesis, Pennsylvania State University, University Park, March 1966.
- Chung, D. H., and W. R. Buessem, The Voigt-Reuss-Hill approximation and elastic moduli of polycrystalline MgO, CaF<sub>2</sub>,  $\beta$ -ZnS, ZnSe, and CdTe, *J. Appl. Phys.*, **38**, 2535, 1967. (See Table 1 on page 2536.)
- Chung, D. H., and Gene Simmons, The pressure and temperature dependence of the isotropic elastic moduli of polycrystalline alumina, *J. Appl. Phys.*, **39**, 5316, 1968.
- Overton, W. C., Relation between ultrasonically measured properties and the coefficients in the solid equation of state, *J. Chem. Phys.*, **37**, 116, 1962. (See equation 7 on page 117.)
- Schreiber, E., and O. L. Anderson, Revised data on polycrystalline magnesium oxide, *J. Geophys. Res.*, **73**, 2837, 1968.
- Soga, N., and O. L. Anderson, High-temperature elastic properties of polycrystalline MgO and Al<sub>2</sub>O<sub>3</sub>, *J. Am. Ceram. Soc.*, **49**, 355, 1966.
- Tagai, H., T. Zisner, T. Mori, and E. Yasuda, Preferred orientation in hot-pressed magnesia, *J. Am. Ceram. Soc.*, **50**, 550, 1967.

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