

Pressure Dependence of the Elastic Constants of Single-Crystalline Magnesium Oxide

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New precision measurements have been made of the pressure dependence of the elastic constants of MgO single crystals by using the ultrasonic pulse superposition method in connection with an automatic peak finder. The results for the first pressure derivatives of the elastic constants lie mostly between the earlier data of Bogardus and the data of Anderson and Andreatch and essentially agree, within the joint experimental error, with both sets of values.

The pressure dependence of the elastic constants of single-crystalline magnesium oxide (MgO) has been measured by several authors [Susse, 1961; Bogardus, 1965; Anderson and Andreatch, 1966]; however, there are some discrepancies among these values. Because of the importance of magnesium oxide as a major constituent of the mantle, it is highly desirable to obtain more accurate values of the elastic constants and their pressure dependences. In addition, magnesium oxide is of interest because of many high-temperature applications and because of its chemical stability in the atmosphere, which makes MgO useful as a standard for the elastic constants and their pressure derivatives.

For these reasons, new measurements were made with an improved experimental technique and increased experimental accuracy by using one of the six specimens of Bogardus [1965]. The purpose of this note is to report the results and to present a careful evaluation of the total experimental error.

The elastic constants of magnesium oxide were determined from ultrasonic velocity measurements as a function of hydrostatic pressure up to 10 kb. The pulse-superposition method of McSkimin [1961] was used with an automatic peak finder constructed by Miller [1969] according to the principles put forth by McSkimin [1965] and McSkimin and Andreatch [1967]. Ultrasonic wave pulses were generated and received with X-cut and ac-cut quartz transducers of 0.35-inch diameter with a resonance frequency of 20 MHz. The pressure was deter-

mined by measuring the resistance change of a manganin cell with a Carey-Foster type bridge obtained from the Harwood Engineering Co., Walpole, Massachusetts. The temperature of the specimen was monitored with a thermocouple, and the measured values of the repetition rate frequency were converted to 25°C by using values for the temperature coefficients of the elastic constants that had been determined with the same ultrasonic interferometer.

The specimen was identical with one of the crystals used by Bogardus [1965]. It was prepared from a larger single-crystalline specimen (purchased from the Norton Co.), which had been obtained by cooling from the melt. Only minor traces of Si, Al, Ca, and Fe could be found by qualitative spectrochemical analysis. The density was measured as 3.579 g/cm³ and agrees well with the X-ray density of 3.581 calculated from the lattice constant of 4.213 Å reported by Swanson and Tatge [1953]. The faces of the specimen were oriented to within 15 min in the directions [110], $\bar{1}\bar{1}0$, and [001], and the respective dimensions are 11.5 × 11.2 × 14.2 mm.

Measurements were made for four wave modes, the three pure modes with propagation in the [110] direction and the longitudinal mode propagating in the [001] direction. This procedure permits one internal check among the data. The relation between $\rho_0 W^2$ (where ρ_0 denotes the initial density and W the natural velocity introduced by Thurston and Brugger [1964]) and pressure, shown in Figure 1, can be seen to be linear. A least-squares method was used to determine the three second-order adia-

batic elastic constants and their isothermal pressure derivatives by using the formulas given by *Thurston and Brugger* [1964]. The standard error was calculated from the mean-square deviation, and the total error was determined by including an estimated error of 0.1 and 1.0% for the density and pressure, respectively. The elastic constants and their pressure derivatives were also converted to purely isothermal and purely adiabatic conditions by using the standard formulas [*Voigt*, 1910; *Barsch*, 1967] and the thermal and thermoelastic data tabulated by *Barsch and Chang* [1967]. The results are listed in Table 1 together with the values for the shear modulus $c_s = \frac{1}{2}(c_{11} - c_{12})$ and for the bulk modulus K . The second-order elastic constant data are in good agreement with the values of *Bogardus* [1965] and *Anderson and Andreatch* [1966]. Also included in Table 1 are the results reported by these investigators for

the isothermal pressure derivatives of the adiabatic elastic constants.

The data reported as the values of *Bogardus* were calculated from the measurements under hydrostatic pressure, which are given in Table IV of *Bogardus* [1965] and have been published before [*Barsch and Chang*, 1967]. The value for the pressure coefficient of the bulk modulus given here differs from the value reported by *Bogardus* [1965] because of a numerical error in that paper and because *Bogardus* used the measurements under uniaxial stress in addition to the values under hydrostatic pressure. The values for the pressure coefficient of the bulk modulus listed in Table IX of *Bogardus* [1965] were calculated from the equation $(\partial K^*/\partial p) = -(1/9K)(c_{111} + 6c_{112} + 2c_{122}) + 1$, where $K^* = V_0(\partial p/\partial V)$ is the bulk modulus with reference to the initial volume V_0 , and c_{111} , c_{112} , and c_{122} are third-order elastic constants. Since

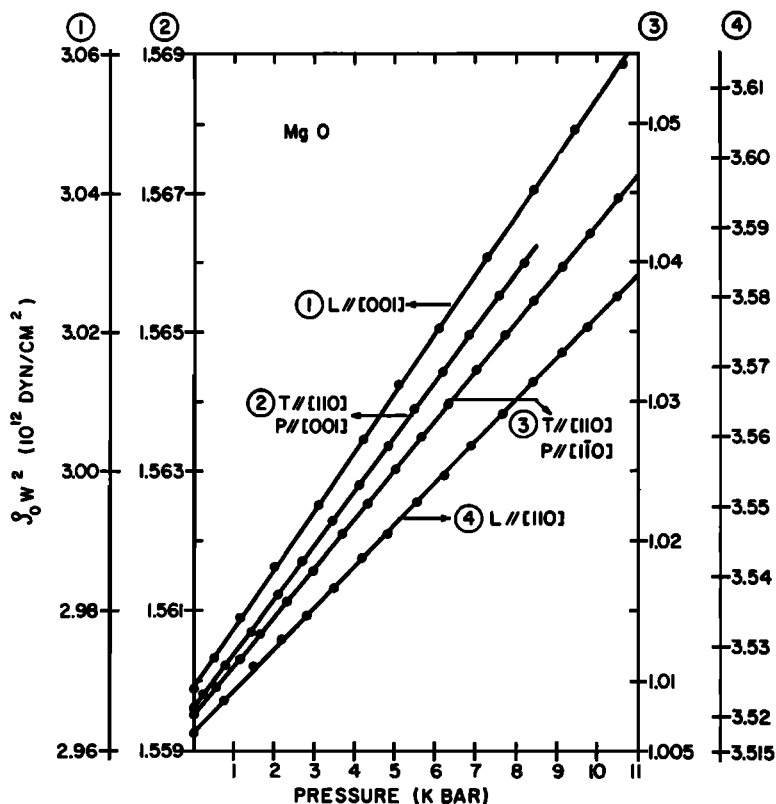


Fig. 1. $\rho_0 W^2$ versus pressure for MgO. L and T denote longitudinal and transverse waves, respectively; P denotes the direction of particle motion.

TABLE 1. Second-Order Elastic Constants (in 10^{11} dynes/cm²) of MgO and Their Pressure Derivatives (Dimensionless) at Zero Pressure

$c_s = \frac{1}{2}(c_{11} - c_{12})$; K = bulk modulus; S and T denote adiabatic and isothermal conditions, respectively ($\rho_0 = 3.579$ g/cm³, $T = 25^\circ\text{C}$).

M	c_{11}	c_{12}	c_{44}	c_s	K	Reference
M^S	29.664	9.508	15.581	10.078	16.226	Present work
	± 0.030	± 0.011	± 0.016	± 0.010	± 0.017	
M^T	29.404	9.248	15.581	10.078	15.967	Present work
$(\partial M^S/\partial p)_S$	8.98	1.84	1.09	3.57	4.22	Present work
$(\partial M^S/\partial p)_T$	1.03	3.34	...	Susse [1961]
	8.93	1.76	1.20	3.59	4.16	Calculated from Bogardus [1965]
	9.477	1.992	1.160	3.743	4.497	Anderson and Andreatch [1966] (at 23°C)
	9.16	1.82	1.12	3.67	4.27	Present work
$(\partial M^T/\partial p)_T$	± 0.10	± 0.09	± 0.06	± 0.06	± 0.08	Present work
	9.18	1.84	1.12	3.67	4.29	

the pressure derivative of the bulk modulus $K = -V(\partial p/\partial V)$, with reference to the instantaneous volume V , is given by $(\partial K/\partial p) = (\partial K^*/\partial p) - 1$, the values reported in Table IX of the Bogardus paper should be decreased by 1, giving, for example, $(\partial K/\partial p) = 3.8$ for MgO.

For $(\partial c_{12}/\partial p)$, $(\partial c_{44}/\partial p)$, and $(\partial c_s/\partial p)$, the results of the present work agree within the combined experimental error with both the data calculated from the measurements of Bogardus [1965] and the results of Anderson and Andreatch [1966], if it is assumed that all three sets of data are subject to the same experimental error that is reported for the results of the present work. For $(\partial c_{11}/\partial p)$ and $(\partial K/\partial p)$ the discrepancy is larger than this combined experimental error. With the exception of

$(\partial c_{44}/\partial p)$, all results of the present work lie between those of Bogardus [1965] and those of Anderson and Andreatch [1966]. The values reported by Susse [1961] for $(\partial c_{44}/\partial p)$ and $(\partial c_s/\partial p)$ are considerably smaller than any of the other values.

The three linear combinations of the intermediate third-order elastic constants, which can be determined from the isothermal pressure derivatives of the adiabatic elastic constants, are given in Table 2. Again, the values calculated from the measurements of Bogardus [1965] are based on his hydrostatic data only. The data given in the first line are based on the individual third-order elastic constants listed in Table V of Bogardus [1965], which were calculated by neglecting the difference between the adiabatic and isothermal bulk moduli. It is apparent that the effect of this approximation together with the inclusion of the measurements under uniaxial stress is especially pronounced for c_s .

TABLE 2. Linear Combinations of the Adiabatic-Isothermal Third-Order Elastic Constants (in 10^{11} dynes/cm²) of MgO

$c_a = c_{111} + 2c_{112}$, $c_b = 2c_{121} + c_{122}$, and $c_c = c_{441} + 2c_{461}$ ($T = 25^\circ\text{C}$).

c_a	c_b	c_c	Reference
-508.5	-25.9	-120.5	Bogardus [1965]
-506.0	-46.0	-121.1	Calculated from Bogardus [1965]
-532.0	-57.1	-119.1	Anderson and Andreatch [1966] (at 23°C)
-516.2	-48.8	-117.3	Present work
± 4.8	± 4.5	± 2.7	

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