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Elastic Constants of Single-Crystal Forsterite as a Function of Temperature and Pressure

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The nine adiabatic elastic stiffness constants of single-crystal forsterite (Mg_2SiO_4) have been measured as a function of hydrostatic pressure and temperature using a pulse superposition technique. The pressure dependence was linear, within experimental error, for all nine coefficients up to 10 kb. Temperature measurements were made in the range from 300° to 700°K. At lower temperatures some curvature was present, but above 500°K the data were linear. The nine adiabatic stiffnesses and their isothermal pressure derivatives at 25°C are presented, and the isobaric temperature derivatives are given at zero pressure in the high temperature limit above 500°K. The elastic constants and their pressure derivatives agree approximately with theoretical data for a hexagonal close-packed structure of oxygen anions assuming only nearest neighbor interactions and central forces. This agreement indicates that the elastic properties of forsterite are predominantly determined by the oxygen anion framework. In addition, the results were used to calculate the isothermal pressure dependence of the volume and of the lattice parameters of forsterite at high pressure from the Murnaghan and Birch equations of state.

INTRODUCTION

Olivine, $(Mg,Fe)_2SiO_4$, has long been proposed to be a dominant constituent of the upper mantle. Estimates of upper mantle composition have been previously based on evidence from terrestrial materials that are considered to be either directly or indirectly derived from the upper mantle, such as ultramafic rocks, olivine nodules from basalts, and garnet peridotite nodules from kimberlites. Additional evidence is obtained from meteorite compositions and from solar and stellar abundances. The most characteristic feature of compositional models is the dominance of olivine as a major component [*Harris et al.*, 1967; *Ringwood*, 1966]. Since an average of twenty-seven published analyses of olivine nodules [*Reay*, 1965] yielded an iron oxide to magnesium oxide ratio of 0.222, compositions near the forsterite (Mg_2SiO_4) end of the olivine solid solution series are of primary importance. The objective of this paper is to present experimental data of the elastic constants for a single-crystal of pure forsterite as a function of pressure to 10 kb and of temperature from 25° to 400°C. These data will be used in a subsequent paper to interpret seismic velocity versus depth profiles in terms of compositional models for the earth's mantle. In this paper the experimental results are applied to the calculation of the isothermal equation of state at high pressure and to the calculation of the pressure dependence of the lattice parameters. These quantities are also of interest in geophysics and crystallography.

In addition to their geophysical relevance, the elastic constants and their dependence on pressure and temperature are also of considerable interest to solid state physics because of the information on the interatomic forces they provide. In fact, the results presented here indicate that the elastic properties of forsterite are primarily determined by the framework of oxygen ions that form a distorted hexagonal close-packed structure, and confirm earlier suggestions that, in general, the elastic properties of oxides with comparatively small cations are quite independent of the nature of the cations [*O. L. Anderson*, 1965; *Gieske and Barsch*, 1968].

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The single-crystal elastic constants and their pressure dependence have been measured so far for a variety of possible earth-forming materials and are reviewed by *O. L. Anderson et al.* [1968]. Prior to this investigation, the elastic constants for a single-crystal of peridot were measured at ambient conditions by *Verma* [1960]. In addition, ultrasonic data for a polycrystalline aggregate of forsterite as a function of hydrostatic pressure to 2 kb has been reported by *Schreiber and Anderson* [1967], and shock wave data for forsterite polycrystals have been presented by *D. L. Anderson and Kanamori* [1968]. While this investigation was in progress, the elastic constants of a single-crystal specimen of forsterite and a single-crystal natural peridot were independently measured by *Kumazawa and Anderson* [1969], as a function of pressure and temperature. In almost all cases, the results of that study are reasonably consistent with those of the present investigation.

EXPERIMENTAL PROCEDURE

Forsterite single-crystals of sufficient size for the measurement of elastic constants may be grown by the flame fusion (Verneuil) technique [*Shankland*, 1967]. The single-crystal boule used in this study was obtained from the Linde Crystal Products Division of the Union Carbide Corporation. Its density was determined to be 3.221_7 g/cm^3 at 25°C. A chemical analysis was carried out by J. B. Bodkin of the Pennsylvania State University Mineral Constitution Laboratory. The results of this investigation, compared with the appropriate values for ideal forsterite, are (in weight per cent):

Oxide, wt %	Specimen	Ideal Mg_2SiO_4
SiO_2	42.82	42.69
MgO	57.16	57.31
CaO	<0.01	...
	99.99%	100.00%

In addition, spectroscopic analysis revealed trace amounts (<200 ppm) of Al and Cu. The original boule was approximately 4½ cm in length, 1½ cm in diameter, and was colorless and transparent to visible light. All measurements were carried out on two samples cut from the original boule.

The adiabatic elastic stiffness coefficients as a function of temperature and pressure were determined by measuring ultrasonic wave velocities using the pulse superposition method of *McSkimin* [1961]. The pressure apparatus has been described previously [*Bogardus*, 1965]. Pressure was measured using a pressure-sensitive manganin resistance cell in conjunction with a Carey-Foster pressure measuring bridge (Model C, Harwood Engineering Company, Walpole, Massachusetts). At 10 kb, the accuracy of the pressure reading is ±0.5%. The adiabatic elastic stiffness coefficients and their pressure dependence were determined at 25.0 ± 0.1°C. The temperature of the pressure chamber and the specimen at equilibrium was monitored using two chromel-alumel thermocouples; the thermal emf was measured on a Leeds and Northrup type K-3 universal potentiometer. The pressure vessel was equipped with an internal furnace, consisting of a coil of Kanthal wire, and was used for the measurements of the elastic coefficients up to temperatures of 450°C.

In order to determine the nine elastic constants of forsterite, several crystallographic orientations are necessary in which the ultrasonic velocities are measured. The prescribed orientations were determined to within 0.5° using a Laüe back-reflection X-ray camera. All faces were ground and polished flat to within 0.0001 cm and parallel to within 0.0001 cm/cm. In order to obtain all the required orientations it was necessary to cut two samples from the original boule; these are designated A and B.

Natural quartz AC-cut and X-cut piezoelectric transducers of 0.89 cm in diameter and a resonance frequency of 20 MHz ± 1% (purchased from the Valpey Corporation, Holliston, Massachusetts) were used to generate and receive the transverse and longitudinal ultrasonic wave pulses. They were cemented to the forsterite sample face with phenyl salicylate for measurement of the adiabatic stiffness coefficients, with Nonaq stopcock grease (Fisher Scientific Company) for the pressure measurements, and with Silastic RTV 891 (a silicone rubber cement) for the temperature measurements.

EXPERIMENTAL RESULTS

The elastic stiffness coefficients at 1 atmosphere, 25°C. Forsterite belongs to the orthorhombic space group Pbnm. Therefore, 9 second-