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THE COMPRESSIBILITY OF FORSTERITE UP TO 300 kbar MEASURED WITH SYNCHROTRON RADIATION

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The effect of pressure on the lattice constants and therefore the volume of synthetic forsterite was determined by energy-dispersive X-ray diffraction from polycrystalline material using synchrotron radiation from the storage-ring DORIS at the HASYLAB, DESY (Hamburg). Pressures up to 300 kbar were applied with a diamond-anvil cell. The pressures were calculated from the volume compression by internal standard method using MgO, Fe and NaCl as pressure calibrants. The isothermal bulk modulus K_0 and also its first pressure derivative K_0' (at 25°C) of forsterite have both been obtained from the experimental data with the Murnaghan equation of state by a two parameter fit yielding $K_0 = 1357(10)$ kbar and $K_0' = 3.98(10)$ (standard deviations in parentheses). We found no differences with the different marker.

1. Introduction

Olivines are considered to be the principal constituents of the upper mantle in the earth (Birch [1], Ringwood [2]). For a better understanding of seismic data and also for the general study of the structure of the earth's interior, the elastic constants of the constituent minerals, e.g. of the olivines, must be known. For forsterite, the Mg-endmember of the olivines, the isothermal compression was measured several years ago by Olinger and Halleck [3] and again by Olinger [4] on polycrystalline material up to 100 kbar and by Hazen [5] on a single crystal up to 50 kbar. Graham and Barsch [6] measured the compression modulus up to 10 kbar using a pulse superposition technique. In all measurements only the compression modul K_0 was determined. In order to calculate not only K_0, but also K_0' of the Murnaghan equation with the necessary reliability it is imperative to determine the p–V data to much higher pressures. For this reason we have remeasured the compressibility of forsterite up to 300 kbar and here we wish to report these results.

2. Experimental

The compressibility was derived from X-ray diffraction data on polycrystalline synthetic material with energy dispersive techniques. For higher accuracy and better resolution in the diffraction diagrams we used synchrotron radiation from the DORIS storage ring at the DESY, Hamburg. Synchrotron radiation is extremely well collimated (divergence about 0.1 mrad), thus improving the resolution by a factor of at least two. Furthermore, the intensity is about four orders of magnitude larger than from sealed X-ray tubes. Typical exposures times are 10 min with synchrotron radiation compared to about 8 h with an X-ray tube. The conditions for the experiments here were $2\theta = 11°$, exposures times $t =$ 500–1500 s.

For the high pressure conditions we used an opposed diamond anvil device according to Piermarini [7] built in this laboratory. The sample in a gasket is placed between the flat, parallel faces of two diamonds, 300 μm in diameter. The pressure was calculated by the internal standard method using successively MgO, Fe and NaCl as markers. Forsterite and one pressure calibrant were finely powdered to 1–2 μm grain size, intimately mixed and immersed in a methanol–ethanol–mixture 4:1. Thus a hydrostatic or at least nearly hydrostatic environment is obtained. The gasket material was an inconel foil of 280 μm original thickness with a hole of 150 μm diameter.

The evaluation of the data was done by profile analysis (Will et al. [8], Lauterjung et al. [9])

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yielding d_{hkl}-values and intensities. The profile-analyzed data were first used to calculate the lattice constants of the marker in order to determine the pressure in the cell, then for the forsterite in order to calculate the compressibility. With three different markers we could check the results against each other, and therefore we obtained high reliability. The different markers also served the purpose of checking whether the compressibility data would show inconsistencies, as has been reported before (Will et al. [10], Bell et al. [11], Sato et al. [12]).

3. Results

Forsterite crystallizes in the orthorhombic system, space group D_{2h}^{16}–Pbnm, with four formula units Mg_2SiO_4 in the unit cell. The diffraction diagrams (fig. 1 shows a representative example) have sufficiently resolved peaks to allow the three lattice constants a_0, b_0 and c_0 to be calculated independently by least squares analysis. Up to 23 reflections ($d_{obs}(\min) = 1.35$ Å) were used. The results are shown in table I. Fig. 2 shows the combined results of the compressibility of forsterite in the form of V_P/V_0 values vs pressure. The Murnaghan equation

$$p = \frac{K_0}{K_0'}\left[\left(\frac{V_0}{V}\right)^{K_0'} - 1\right], \tag{1}$$

with $K_0 = -V(\partial p/\partial V)_T$ and $K_0' = [(\partial K/\partial p)_T]_{p=0}$, was fitted to the measured data, yielding K_0 and K_0'. We have calculated these two constants independently for the three markers (table II), and also by combining the three data sets as shown in fig. 2. The final result is $K_0 = 1357$ (10) kbar $K_0' = 3.98$ (10).

4. Discussion

One specific purpose of this experimenal series was to reliably establish the bulk-moduli K_0 and K_0' of forsterite by using different markers. As has

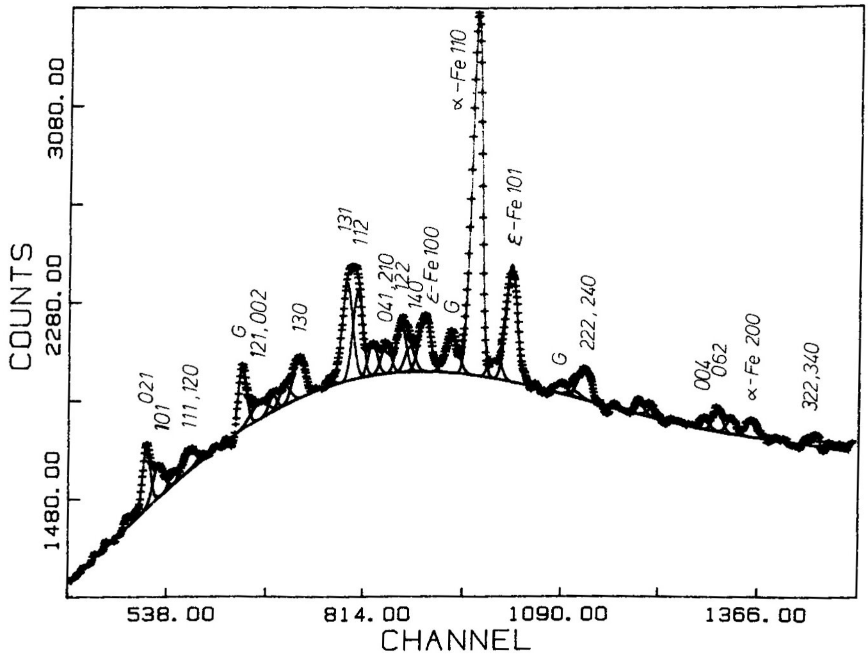

Fig. 1. Diffraction diagram of forsterite with Fe as a marker measured by energy dispersion with synchrotron radiation. $2\theta = 10.71°$, $p = 98.0$ kbar, $t = 1500$ s. G stands for gasket.

Table I
Variation of lattice constants a_p, b_p, c_p and the compression V/V_0 with increasing pressure. The respective internal markers for pressure calibration are indicated. The average standard deviations are 0.011, 0.022 and 0.012 for a_p, b_p and c_p respectively

P (kbar)	σ_P (kbar)	Marker	a_p	b_p	c_p	V/V_0	σ_{V/V_0}
0.0	0.0		4.757	10.195	5.982	1.0000	0.0
3.8	0.9	NaCl	4.749	10.185	5.971	0.9953	0.0035
13.7	1.4	Fe	4.741	10.160	5.958	0.9883	0.0026
20.5	0.8	Fe	4.766	10.107	5.954	0.9877	0.0030
27.1	2.5	MgO	4.754	10.127	5.943	0.9843	0.0052
35.1	2.5	NaCl	4.730	10.080	5.927	0.9738	0.0033
38.8	0.1	Fe	4.744	10.080	5.942	0.9787	0.0032
47.3	4.0	MgO	4.747	10.005	5.903	0.9646	0.0056
47.4	3.4	NaCl	4.721	10.067	5.928	0.9708	0.0048
47.8	1.9	Fe	4.731	10.094	5.918	0.9735	0.0031
69.2	2.9	Fe	4.725	9.984	5.892	0.9573	0.0028
75.2	5.7	MgO	4.720	9.982	5.886	0.9541	0.0046
98.0	4.5	Fe	4.671	9.928	5.841	0.9330	0.0031
108.6	4.6	NaCl	4.697	9.884	5.834	0.9331	0.0064
116.7	7.7	MgO	4.673	9.870	5.800	0.9202	0.0048
127.6	2.7	Fe	4.681	9.860	5.798	0.9218	0.0038
156.4	5.5	NaCl	4.655	9.811	5.782	0.9098	0.0066
156.8	2.1	MgO	4.649	9.813	5.792	0.9090	0.0054
164.5	0.9	Fe	4.668	9.781	5.739	0.9012	0.0045
174.2	2.6	MgO	4.689	9.728	5.771	0.9056	0.0060
208.3	1.4	Fe	4.632	9.699	5.757	0.8909	0.0050
223.7	0.9	MgO	4.620	9.707	5.743	0.8859	0.0059
272.4	1.8	MgO	4.596	9.588	5.702	0.8643	0.0044
293.4	1.2	MgO	4.605	9.563	5.630	0.8529	0.0041
295.1	4.9	Fe	4.629	9.551	5.612	0.8547	0.0035

been demonstrated, we found good agreement for all markers in the pressure range up to 300 kbar. This seems especially noteworthy, since in several previous publications, for example Will et al. [10], or Bell et al. [11], or Sato et al. [12], such inconsistencies were reported.

The compressibility value K_0 determined here is larger in magnitude than the value originally determined by Graham and Barsch [6] from ultrasonic data ($K_0 = 1280$ kbar, $K_0' = 5.0$) in the pressure range up to only 10 kbar. The values were also later duplicated by Kumazawa and Anderson [13] by ultrasonic measurements ($K_0 = 1260$ kbar, $K_0' = 5.3$–5.4). They are also

Table II
Bulk-moduli of forsterite and their pressure derivatives for the different markers compared with literature values

Marker (K_0 in kbar)		K_0 (kbar)	K_0'	P_{max} (kbar)	Method
Fe ($K_0 = 1640$)	Present work	1349 (16)	4.00 (17)	300	static compression (X-rays)
MgO ($K_0 = 1560$)		1361 (17)	3.98 (17)	300	
NaCl ($K_0 = 260$)		1364 (15)	3.98 (24)	150	
All data combined		1357 (10)	3.98 (10)	300	
Olinger [4]		1200	5.6	100	static compression
Graham and Barsch [6]		1280	5.0	10	ultrasonic
Hazen [5]		1350	4.0	50	static compression (single crystal)

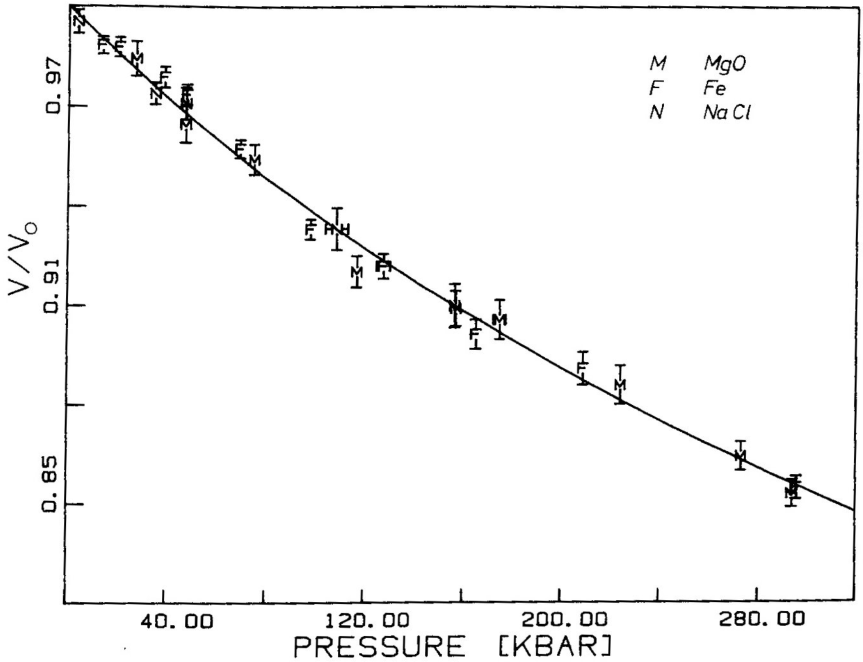

Fig. 2. Compressibility of forsterite plotted as V_p/V_0 versus pressure. The markers are symbolized as indicated. The solid curve describes the fit of the Murnaghan equation to the measured data.

larger than the values determined by Olinger [4] from static compression data ($K_0 = 1200$ kbar, $K_0' = 5.6$) up to 100 kbar.

The best results were obtained by a two parameter fit of our data to the Murnagham equation, giving $K_0 = 1357$ (10) kbar and $K_0' = 3.98$ (10). Since the decisive parameter in the Murnaghan equation is K_0', which is difficult to measure, the differences in the data sets are due to the differences of K_0', which in all previous publications have arbitrarily been set constant to the mentioned values. Therefore, for the determination of K_0' compression data to rather high pressures are needed. Only by having such data up to high pressures was it possible for us to obtain convergence with a two parameter fit of the Murnaghan equation.

In order to gain some understanding of the literature data especially on K_0', we have tried to calculate the pressure derivative K_0' from the data published by Olinger [4] by a two parameter fit. When both parameters K_0 and K_0' were varied simultaneously, the result was a negative value for K_0'. We consider therefore this as evidence that the compressibility should be measured to pressures as high as possible in order to determine reliable values of K_0'. Our results are in agreement with the single crystal measurements of Hazen [5] who fixed K_0' in accordance with finite strain theory at 4.0.

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References

[1] F. Birch, J. Geophys. Res. 57 (1952) 227.
[2] A.E. Ringwood, Composition and Petrology of the Earth's Mantle (McGraw-Hall, New York, 1975).
[3] B. Olinger and P.M. Halleck, J. Geophys. Res. 79 (1974) 5535.
[4] B. Olinger, in: High-Pressure Research: Applications in Geophysics, eds. M.H. Manghnani and S. Akimoto (Academic, New York, 1977) p. 325.

[5] R.M. Hazen, Am. Mineral. 61 (1976) 1280.

[6] E.K. Graham and G.R. Barsch, J. Geophys. Res. 74 (1969) 5949.

[7] G.J. Piermarini, S. Block and J.D. Barnett, J. Appl. Phys. 44 (1973) 5377.

[8] G. Will, W. Parrish and T. Huang, Appl. Cryst. 14 (1982) 483.

[9] J. Lauterjung, E. Hinze and G. Will, Nucl. Instr. and Meth. (1985) in press.

[10] G. Will, E. Hinze and W. Nuding, in: High-Pressure Researches in Geosciences (E. Schweizerbart'sche Verlagsbuchhandlung, Stuttgart, 1982) p. 177.

[11] F. Bell, H.K. Mao and J.L. England, Carnegie Inst. Washington Year Book (1971) p. 277.

[12] Y. Sato, T. Yagi, Y. Ida and S. Akimoto, High Temp.–High Press. 7 (1975) 315.

[13] M. Kumazawa and O.L. Anderson, J. Geophys. Res. 74 (1969) 5961.