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ON THE EQUATIONS OF STATE OF HIGH-PRESSURE SOLID PHASES

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A practical scheme by which one can construct equations of state of high-pressure solid phases that cannot be determined experimentally given the present state of technology, is proposed and illustrated with three examples for its possible application to the study of elasticity and the constitution of the earth's mantle.

1. Introduction

Most of the known mantle minerals found at ambient conditions undergo one or more phase changes in the pressure and temperature field of the earth's interior. Finding the proper equations of state of solids before and after a phase change is essential in the interpretation of geophysical field observations as well as in our understanding of solid-state properties of these materials. The bulk modulus K and its first derivative with respect to pressure $(\mathrm{d}K/\mathrm{d}p)$ are the important parameters entering into equations describing the pressure-volume relationship of the solid [1]. Laboratory measurements of these equation-of-state (EOS) parameters for solid phases found at ambient conditions are now routine procedures in most ultrasonic-pressure laboratories. For solid phases that exist at high pressures, however, such measurements cannot be made given the present state of technology. The purpose of this communication is to suggest a practical scheme by which one can estimate values of these EOS parameters of high-pressure phases and then to illustrate the scheme with three examples.

2. Scheme

Using Birch's law [2] to estimate velocities of elastic waves in a mineral undergoing compression is now well-known [3, 4]. Chung [3] using Birch's law, has also estimated velocities of compressional (V_p), shear (V_s) and bulk (V_ϕ) waves in the olivine-transformed spinels. Since the adiabatic bulk modulus K_s is related to density ρ and the bulk sound velocity V_ϕ as

$$K_s = \rho\, V_\phi^2, \tag{1}$$

the K_s value of a solid phase after the phase change can be found. (It is noted that $K_s = K\,(1 + T\alpha\gamma)$, where α is the coefficient of volume expansion, γ Grüneisen's ratio and T the temperature in degrees Kelvin, and that the value of this isothermal bulk modulus K is smaller than that of K_s by a few percent in general.) Thus, the first of the two EOS parameters is found for high-pressure phases in this rather straightforward manner.

The second EOS parameter to be found is $(\mathrm{d}K/\mathrm{d}p)$, which cannot be measured ultrasonically given the present state of technology. It is for this parameter that the author suggests an approximation scheme whereby one can estimate values of $(\partial K_s/\partial p)$ for high-pressure phases.

Recall Birch's law for V_ϕ [4]:

$$V_\phi = a\,(\bar{m}) + b\rho, \tag{2}$$

where $\bar{m}$ is the mean atomic weight and the constants a and b are obtainable from a least-squares fit of experimental values of V_ϕ for substances of similar $\bar{m}$ or for substances of the same $\bar{m}$ as illustrated with periclase by Wang [4]. In view of eqs. (1) and (2), the adiabatic bulk modulus K_s is

$$K_s = \rho\,(a + b\rho)^2. \tag{3}$$

Table 1

Elasticity data of some minerals and rocks with mean atomic weight of 20 to 21.

	$\bar{m}$	ρ (g/cm^3)	V_p (km/sec)	V_ϕ (km/sec)	K_S (mb)	Calculated $\left(\frac{\partial K_S}{\partial p}\right)_S$ Eq. (4)	Calculated Eq. (5)	Measured $\left(\frac{\partial K_S}{\partial p}\right)_T$
rly	21.0	2.674	6.23	4.63	0.573	4.1	5.8	–
rly	21.0	2.672	6.45	4.61	0.568	4.1	5.9	–
port	21.6	2.678	6.51	4.81	0.620	4.0	5.6	–
Mt.	20.7	2.679	6.40	4.63	0.574	4.1	5.8	–
	20.8	2.708	6.39	4.72	0.603	4.0	5.7	–
ar	20.2	2.694	6.76	5.01	0.676	3.9	5.4	–
	20.4	3.223	8.28	6.11	1.203	3.8	4.6	–
er	21.0	3.287	7.78	5.87	1.133	4.0	4.9	–
	20.9	3.346	8.28	6.29	1.324	3.8	4.6	–
	20.9	3.312	8.42	6.31	1.320	3.8	4.6	–
	21.0	3.340	7.820	5.607	1.050	4.2	5.2	–
	21.0	3.380	7.850	5.499	1.022	4.3	5.3	–
	20.1	3.224	8.569	6.316	1.286	3.7	4.5	5.37
	20.1	3.222	8.593	6.330	1.291	3.7	4.5	4.97
	20.1	3.217	8.534	6.309	1.281	3.7	4.5	5.04
, pc	20.6	3.273	8.422	6.245	1.277	3.8	4.6	5.08
, sc	20.7	3.311	8.421	6.252	1.294	3.8	4.6	5.13
, sc	20.9	3.324	8.482	6.227	1.289	3.8	4.6	–
, pc	21.0	3.330	8.317	6.189	1.274	3.9	4.7	5.13
	20.3	3.588	9.715	7.372	1.950	3.6	4.1	–
	20.3	3.588	9.762	7.414	1.972	3.6	4.1	4.20
sc	20.4	3.619	9.914	7.471	2.020	3.6	4.1	4.18
	20.2	3.581	9.847	6.738	1.626	3.8	4.4	4.16
	20.2	3.582	9.692	6.729	1.622	3.8	4.4	4.30
	20.2	3.584	9.692	6.723	1.620	3.8	4.4	4.54
	20.2	3.579	9.661	6.736	1.624	3.8	4.4	4.43
	20.2	3.582	9.692	6.776	1.640	3.8	4.4	4.28
	20.2	3.580	9.691	6.727	1.620	3.8	4.4	4.50
	20.4	3.986	10.847	7.950	2.519	3.7	4.1	–
	20.4	3.986	10.885	7.986	2.542	3.7	4.1	4.27
c	20.4	3.986	10.888	7.920	2.500	3.7	4.1	–
c	20.4	3.972	10.845	7.967	2.521	3.7	4.1	3.98
c	20.4	3.986	10.890	7.999	2.551	3.6	4.0	4.19
	20.0	2.649	6.047	3.778	0.378	4.7	7.3	6.42
	20.0	2.649	6.066	3.773	0.377	4.7	7.4	6.50

o Twin Sisters dunite; sc and pc refer, respectively, to gem-quality single-crystals and synthetic polycrystalline aggregates. The single-cr
t-Reuss-Hill (VRH) values in all cases.