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A new method for thermal pressure using equations of state for MgO

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ABSTRACT

In the present study we have developed a new method for determining thermal pressure in case of MgO using the Kushwah pressure–volume equation along different isotherms at selected temperatures up to 1800 K. The results obtained down to a compression, $V/V_0 = 0.6$, present close agreement with the values determined from the Stacey reciprocal K-primed equation. The present method is based on the idea of using equations of state for variations of pressure with volume to represent variations of pressure with temperature in order to determine values of thermal pressure, which is defined as the pressure that would prevent volume thermal expansion. It has been found that the thermal pressure for MgO depends on temperature as well as compression.

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1. Introduction

In order to understand the behaviour of materials at high pressures and high temperatures, it is necessary to have a precise knowledge of pressure (P)-volume (V)-temperature (T) relationship [1–3]. For this purpose, the most convenient method is based on an equation of state which can be written as

$$P(V,T) = P(V,0) + P_{\mathrm{th}}(V,T) \tag{1}$$

where the first term on right represents the P–V relationship at $T = 0$. Equation of state has been widely used in the field of condensed matter physics, nuclear physics, chemistry, geology, engineering and nanotechnology [4–6].

To understand the phenomenon of thermoelasticity of materials at high temperatures we need accurate values of thermal pressure [7,8]. We can determine thermal pressure using thermal expansivity α and isothermal bulk modulus as a function of both P and T. However, such data are not available mainly because of the limitations of experimental methods used for measurements at high P and high T [9–11]. We develop here a method for determining thermal pressure using a procedure based on the equation of state recently formulated by Stacey [12–14].

2. Method of analysis

The reciprocal K-primed EOS due to Stacey [12] is written as

$$\frac{1}{K'} = \frac{1}{K'_0} = +\left(1 - \frac{K'_\infty}{K'_0}\right)\frac{P}{K} \tag{2}$$

where K_0 and K_0' are respectively the values of bulk modulus K and its pressure derivative $K' = \mathrm{d}K/\mathrm{d}P$, both at $P = 0$. K_∞' is the value of K' at $P \to \infty$, satisfying the algebraic identity [15]

$$\frac{1}{K'_\infty} = \left(\frac{P}{K}\right)_\infty \tag{3}$$

Eq. (2) makes an effective use of Eq. (3). Eq. (2) on successive integrations yields the following expressions

$$K = K_0\left(1 - K'_\infty\frac{P}{K}\right)^{-K'_0/K'_\infty} \tag{4}$$

and

$$\ln\left(\frac{V}{V_0}\right) = \frac{K'_0}{K'^2_\infty}\ln\left(1 - K'_\infty\frac{P}{K}\right) + \left(\frac{K'_0}{K'_\infty} - 1\right)\frac{P}{K} \tag{5}$$

where V_0 is the volume V at initial conditions of pressure and temperature. Eq. (2) on differentiation gives the following relationship at $P = 0$.

$$K_0K''_0 = -K'_0(K'_0 - K'_\infty) \tag{6}$$

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Table 1
Values of input data for MgO on density ρ in gm/cc, volume $V(T,0)$ in cc/mol and isothermal bulk modulus $K_T(T,0)$ in GPa all from Anderson [1] and $K_T'(T,0)$ from Isaak et al. [19].

T(K)	ρ	$V(T,0)$	$K_T(T,0)$	$K_T'(T,0)$
300	3.585	11.24	161.6	4.15
400	3.573	11.28	158.9	4.18
500	3.559	11.32	156.2	4.21
600	3.545	11.37	153.2	4.24
700	3.531	11.41	150.4	4.27
800	3.516	11.46	147.4	4.30
900	3.501	11.51	144.3	4.33
1000	3.486	11.56	141.4	4.36
1100	3.470	11.61	138.3	4.39
1200	3.454	11.67	135.1	4.42
1300	3.438	11.72	132.1	4.46
1400	3.422	11.78	128.9	4.49
1500	3.405	11.84	125.7	4.53
1600	3.388	11.90	122.5	4.57
1700	3.371	11.96	119.6	4.61
1800	3.354	12.02	116.6	4.65

where K_0'' is the value of second pressure derivative of bulk modulus, i.e., $K'' = \mathrm{d}^2K/\mathrm{d}P^2$ at $P = 0$. Equations (2), (4) and (5) have been found to yield excellent fits for the seismic data in case of the Earth lower mantle and core [13,14] as well as for a variety of solids [16–18]. In all these studies the fitted values of K_∞' are considerably larger than 5/3, thus satisfying the thermodynamic constraint $K_\infty' > 5/3$ found by Stacey [12]. The following empirical relationship has been found to hold good [13,14,16–18].

$$K_\infty' = 0.6K_0' \tag{7}$$

Recently Shrivastava [17] has demonstrated that the Kushwah EOS [16] yields close agreement with the Stacey EOS for different metals up to very high compressions. The generalized Kushwah logarithmic EOS can be written as [16].

$$P(1-x)^{K_\infty'} = A_1\ln(1+x) + A_2\{\ln(1+x)\}^2 + A_3\{\ln(1+x)\}^3 \tag{8}$$

where $x = (1 - V/V_0)$, V_0 is the volume at $P = 0$. The constants A_1, A_2 and A_3 are determined by using the conditions at $P = 0$ [16]

$$\begin{aligned} A_1 &= K_0 \\ A_2 &= \tfrac{K_0}{2}\left(K_0' - 2K_\infty' + 2\right) \\ &\text{and} \\ A_3 &= \tfrac{K_0}{6}\left(K_0K_0'' + K_0'^2 - 3K_\infty'K_0' + 6K_0' + 3K_\infty'^2 - 12K_\infty' + 6\right) \end{aligned} \tag{9}$$

The parameters A_1, A_2 and A_3 are determined using K_0, K_0', K_0K_0'' and K_∞'. The results obtained for hcp iron with the help of Eq. (8) have been found to be identical with those derived from the Stacey reciprocal K-primed EOS. The parameters for hcp iron, $K_0 = 170$ GPa, $K_0' = 4.98$, $K_\infty' = 3.0$ and $K_0K_0'' = -9.86$ taken in Eq. (9) were exactly the same as used for the Stacey EOS. Values of K_0K_0'' and K_∞' were determined from Eqs. (6) and (7). Thus the Kushwah EOS is very similar with the Stacey EOS. It should be mentioned that for determining P–V relationship with the help of the Stacey EOS, Eq. (5), we need the values of bulk modulus K at elevated pressures. On the other hand, the Kushwah EOS, Eq. (8) can be used conveniently with the help of zero pressure value of bulk modulus in order to find pressure as a function of volume V.

3. Results and discussions

In the present study, we use Eq. (8) to determine values of thermal pressure for MgO at different temperatures and volumes. MgO (periclase) is one of the most common materials in the Earth science, Physics, and Chemistry. The difference in thermal pressure ΔP_{th} at two temperatures is defined as follows [1].

$$\Delta P_{th} = P(V,T) - P(V,T_0) \tag{10}$$

Table 2
Pressure-volume-temperature relationship for MgO. The results are determined from the Kushwah EOS (Eq. (8)) mimicking the Stacey reciprocal K-primed EOS (Eq. (5)).

Volume V(cc/mol)	Pressure P(GPa) at different temperatures															
	300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
11.24	0.00	0.57	1.12	1.81	2.33	2.98	3.60	4.22	4.81	5.51	6.06	6.71	7.34	7.95	8.54	9.12
10.74	8.08	8.63	9.17	9.84	10.34	10.98	11.58	12.18	12.74	13.43	13.96	14.59	15.20	15.78	16.36	16.92
10.24	18.21	18.75	19.27	19.94	20.40	21.02	21.60	22.19	22.71	23.39	23.88	24.49	25.08	25.63	26.18	26.73
9.74	30.96	31.48	31.98	32.63	33.06	33.66	34.21	34.77	35.26	35.91	36.37	36.94	37.50	38.01	38.54	39.06
9.24	47.03	47.53	48.01	48.66	49.04	49.62	50.13	50.67	51.09	51.72	52.14	52.66	53.18	53.65	54.14	54.63
8.74	67.42	67.91	68.36	68.99	69.33	69.88	70.34	70.84	71.20	71.79	72.16	72.63	73.10	73.51	73.96	74.41
8.24	93.48	93.94	94.37	94.99	95.27	95.79	96.19	96.65	96.92	97.46	97.78	98.17	98.58	98.91	99.32	99.72
7.74	127.08	127.53	127.93	128.55	128.75	129.23	129.55	129.97	130.13	130.61	130.86	131.14	131.49	131.73	132.07	132.42
7.24	170.92	171.36	171.73	172.20	172.45	172.89	173.11	173.34	173.50	173.67	174.00	174.21	174.37	174.59	174.85	175.13
6.74	228.88	229.32	229.66	230.00	230.28	230.66	230.76	230.81	230.89	231.02	231.10	231.22	231.30	231.41	231.50	231.68

Table 3
Values of thermal pressure ΔP_{th} determined from Eq. (10) using the results given in Table 2.

Volume V(cc/mol)	Thermal pressure ΔP_{th}(GPa) at different temperatures															
	300 K	400 K	500 K	600 K	700 K	800 K	900 K	1000 K	1100 K	1200 K	1300 K	1400 K	1500 K	1600 K	1700 K	1800 K
11.24	0.00	0.57	1.12	1.81	2.33	2.98	3.60	4.22	4.81	5.51	6.06	6.71	7.34	7.95	8.54	9.12
10.74	0.00	0.55	1.09	1.77	2.26	2.90	3.51	4.11	4.67	5.36	5.88	6.52	7.13	7.71	8.29	8.85
10.24	0.00	0.54	1.06	1.72	2.19	2.81	3.39	3.97	4.50	5.17	5.67	6.28	6.86	7.41	7.97	8.51
9.74	0.00	0.52	1.02	1.67	2.10	2.70	3.25	3.82	4.30	4.95	5.41	5.98	6.54	7.05	7.58	8.10
9.24	0.00	0.50	0.98	1.62	2.01	2.59	3.09	3.63	4.06	4.68	5.10	5.63	6.15	6.61	7.11	7.60
8.74	0.00	0.48	0.93	1.57	1.90	2.46	2.91	3.42	3.78	4.37	4.74	5.20	5.68	6.08	6.54	6.99
8.24	0.00	0.46	0.89	1.52	1.79	2.31	2.71	3.17	3.44	3.99	4.30	4.69	5.11	5.44	5.84	6.25
7.74	0.00	0.45	0.85	1.46	1.67	2.15	2.47	2.89	3.05	3.53	3.78	4.06	4.41	4.65	4.99	5.33
7.24	0.00	0.44	0.81	1.28	1.53	1.97	2.19	2.42	2.58	2.75	3.08	3.29	3.45	3.67	3.93	4.21
6.74	0.00	0.43	0.78	1.12	1.39	1.78	1.88	1.93	2.01	2.14	2.22	2.34	2.42	2.53	2.62	2.79

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