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Elastic Constants of Mantle Minerals at High Temperature

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Abstract A simple theoretical model is developed to investigate the temperature dependence of elastic constants. The method is based on a new expression for the temperature dependence of the bulk modulus and the formulation derived from Tallon's model. The proposed relationship is applied to study the elastic constants of the solids of significance to geophysics applications. The calculated values of elastic constants are found to show good agreement with available experimental data.

Keywords Bulk modulus · Elastic constants · High temperatures

1 Introduction

Because of their use in geophysical problems [1], the behavior of elastic constants as a function of temperature has attracted the attention of experimental investigators [2–4] as well as theoreticians [5–8]. The theoretical attempts made in various studies are of two kinds. One methodology depends on the theory of interionic potentials, whereas the other is entirely free from the use of interionic potentials. It has been observed that the methods based on the theory of interionic potentials, either two-body or three-body, are very tedious [5–8], and involve a considerable amount of computational work in addition to various approximations. Thus, it is useful to propose a simple and

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straightforward method for predicting high-temperature elastic constants, which is the purpose of the present paper.

In the present paper, combining a new expression for the temperature dependence of the bulk modulus with the formulation derived from Tallon's model [9], we present elastic constants at high temperature for ten solids, including silicates, oxides, and alkali halides. The results are found to yield close agreement with the available experimental data.

2 Method of Analysis

The isothermal Anderson–Grüneisen parameter connects the thermoelastic and thermodynamic properties in the following way [10]:

$$\delta_T = -\frac{1}{\alpha B_T}\left(\frac{\partial B_T}{\partial T}\right)_P, \tag{1}$$

where α is the volume expansion coefficient or thermal expansivity and B_T is the thermoelastic constant, known as the isothermal bulk modulus.

The mathematical definition of the volume thermal expansion coefficient or the volume thermal expansivity can be expressed as follows:

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P. \tag{2}$$

By using Eqs. 1 and 2, we get

$$\delta_T = -\frac{V}{B_T}\left(\frac{\partial B_T}{\partial V}\right)_P. \tag{3}$$

It is recommended [9] that Eq. 3 can be generalized to be applicable for any elastic modulus. Thus, the following expression represents the generalized form of Eq. 3:

$$\delta_T = -\frac{V_0}{M}\left(\frac{\partial M}{\partial V}\right)_P, \tag{4}$$

where M represents any of the elastic moduli, such as C_{11}, C_{12}, C_{44}, C_S, or B_S. Here C_{11} and C_{12} are the second-order elastic moduli, $C_S = (C_{11} - C_{12})/2$ is the shear modulus, and $B_S = (C_{11} + 2C_{12})/3$ is the adiabatic bulk modulus.

A method to estimate the temperature dependence of the bulk modulus has been developed with approximation that α depends linearly on temperature [11]. But we find that, for the case of NaCl for which experimental results have been reported, the values of B_T calculated in Ref. [11] are adequate for small expansions. The percentage differences increase with increasing temperature and become 9.75 % at the melting point. Thus, the approximation that α depends linearly on temperature is valid only for small expansions that are in the low-temperature range.

Through comparisons and analysis of some experimental data, this paper proposes that α depends quadratically on temperature, which can be written as follows:

$$\alpha = \alpha_0 + \alpha_0' (T - T_0) + \frac{\alpha_0''}{2} (T - T_0)^2 , \tag{5}$$

where α_0 is the value of α at T_0. α_0' and α_0'' are, respectively, the first- and second-order temperature derivatives of α at initial temperature $T = T_0 = 300\,\mathrm{K}$. If one assumes the product αB_T remains constant [12], then we get, from Eq. 1, the following approximate formulation:

$$\delta_T = \frac{1}{\alpha^2} \left(\frac{\partial \alpha}{\partial T} \right)_P . \tag{6}$$

Assuming δ_T to be independent of T [12], we can get the following relations:

$$\alpha_0' = \left(\frac{\partial \alpha}{\partial T} \right)_P = \delta_{T_0} \alpha_0^2 \tag{7}$$

and

$$\alpha_0'' = \left(\frac{\partial^2 \alpha}{\partial T^2} \right)_P = 2\delta_{T_0}^2 \alpha_0^3, \tag{8}$$

where δ_{T_0} is the value of δ_T at T_0 and at atmospheric pressure, i.e., at $P = 0$. So Eq. 5 can be rewritten as follows:

$$\alpha = \alpha_0 + \delta_{T_0} \alpha_0^2 (T - T_0) + \delta_{T_0}^2 \alpha_0^3 (T - T_0)^2 . \tag{9}$$

Substituting the value of α from Eq. 9 in Eq. 1, we get

$$\frac{\mathrm{d}B_T}{B_T} = -\delta_{T_0} [\alpha_0 + \delta_{T_0} \alpha_0^2 (T - T_0) + \delta_{T_0}^2 \alpha_0^3 (T - T_0)^2] \mathrm{d}T. \tag{10}$$

Integrating Eq. 10, we finally get the following expression for $B_T(T)$:

$$\frac{B_T}{B_{T_0}} = \exp\left\{ -\delta_{T_0} \alpha_0 (T - T_0) \left[1 + \frac{1}{2} \delta_{T_0} \alpha_0 (T - T_0) + \frac{1}{3} \delta_{T_0}^2 \alpha_0^2 (T - T_0)^2 \right] \right\} , \tag{11}$$

where B_{T_0} is the value of B_T at initial temperature $T = T_0 = 300\,\mathrm{K}$ and at atmospheric pressure.

Equation 11 may be used to determine the temperature dependence of elastic constants. Following the method of generalization as used by Tallon [9] to get Eq. 4, we can generalize Eq. 11 as follows:

$$\frac{M}{M_0} = \exp\left\{ -\delta_{M_0} \alpha_0 (T - T_0) \left[1 + \frac{1}{2} \delta_{M_0} \alpha_0 (T - T_0) + \frac{1}{3} \delta_{M_0}^2 \alpha_0^2 (T - T_0)^2 \right] \right\} \tag{12}$$

Table 1 Values of input parameters [2]; α_0 in $10^{-6}\ K^{-1}$

	Pyrope-rich garnet	Grossular garnet garnet	$MgAl_2O_4$	MnO	NaCl	Olivine $Fe_{90}Fa_{10}$	Fe_2SiO_4	Mn_2SiO_4	Co_2SiO_4	Al_2O_3
α_0	23.6	19.2	21.1	34.6	118	26.6	26.1	22.7	22.7	16.2
δ 110	5	6.3	6.08	7.4	6.27	3.7	6.2	5.9	4.9	5.8
δ 120	4.5	2.1	5.95	0.061	0.051	6.2	7.2	7.6	7.76	0.56
δ 440	4	5.7	4.7	3.1	2.34	7.4	2.4	8.4	5.4	10.35
δ 220						6.01	8.05	7.2	5.1	
δ 230						3.65	2.65	5.35	6.35	
δ 310						5.4	3.4	6.4	7.6	
δ 330						5.7	7.5	6.1	6.12	4.25
δ 550						6.2	2.2	7.24	7.18	
δ 660						7.64	10.65	10.67	7.65	
δ 130										5.82
δ 140										−5.48

Here δ_{M_0} is given by Eq. 1 as defined by Kumar and Bedi [13]. The values of these constants (δ_{M_0}) are calculated from the measure values of $(\partial M/\partial T)_0$ as given in Table 1 along with the other input data.

3 Results and Discussion

In order to judge the suitability of Eq. 11, we have calculated the values of B_T as a function of temperature and compared the results (Table 2) with experimental data. The results obtained from Ref. [11] are also included in Table 2 for the purpose of comparison. We note that the values of B_T calculated from Eq. 11 are in close agreement with experimental data. Thus, Eq. 11 proposed by the authors seems to be suitable for the temperature dependence of the bulk modulus. Equation 11 may be generalized in the form of Eq. 12. Equation 12 is used to compute the temperature dependence of elastic moduli. We calculated the values of elastic moduli such as C_{11}, C_{12}, C_{44}, C_S, or B_S of ten solids of significance to geophysics. The results thus obtained are given in Tables 3–12 along with the experimental data [2].

The results obtained for the elastic constants for these ten solids under study present reasonably good agreement with the available experimental data [2]. The nature

Table 2 Values of bulk modulus B_T (in kbar) at different temperatures T for NaCl ($\delta_{T_0} = 5.95$ [11])

T (K)	B_T		
	Ref. [11]	This work	Exp. [2]
300	240.0	240.0	240.0
400	219.7	223.2	224.1
500	199.9	206.3	205.0
600	18.09	189.6	188.0
700	151.2	172.9	174.0
800	145.6	156.6	156.0
900	128.8	140.6	140.9
T_m (1,050 K)	107.4	117.5	119.0
Percentage deviation at T_m	9.75 %	1.26 %	

Table 3 Pyrope-rich garnet: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{12}		C_{44}		C_S		B_S	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	296.6	296.6	108.5	108.5	91.6	91.6	94.0	94.0	171.2	171.2
400	293.1	292.7	107.3	106.9	90.7	90.8	92.9	92.9	169.3	168.9
600	286.1	285.5	105.0	104.6	89.0	89.1	90.5	90.5	165.4	164.9
800	279.1	278.5	102.7	102.1	87.3	87.4	88.2	88.0	161.5	161.3
1,000	272.1	271.2	100.4	100.3	85.5	85.5	85.8	85.5	157.7	157.3

Table 4 Grossular garnet: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{12}		C_{44}		C_S		B_S	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	318.9	318.9	92.2	92.2	102.9	102.9	113.4	113.4	167.8	167.8
500	311.9	311.7	91.5	91.5	100.8	100.4	110.2	110.1	164.9	164.9
700	304.9	303.8	90.7	90.5	98.8	98.7	107.1	106.6	162.1	161.6
900	298.0	296.5	90.0	90.2	96.7	96.5	104.0	103.2	159.3	158.9
1,100	291.0	289.1	89.2	89.8	94.7	94.2	100.9	99.7	156.5	156.2
1,300	284.0	280.5	88.5	88.7	92.6	91.8	97.8	96.0	153.7	152.6

Table 5 $MgAl_2O_4$: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{12}		C_{44}		C_S		B_S	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	292.2	292.2	168.7	168.7	156.5	156.5	61.8	61.8	209.9	209.9
400	288.5	288.6	166.6	166.3	154.9	155.3	60.9	61.1	207.2	207.1
600	281.0	281.1	162.3	161.9	151.8	152.2	59.3	59.6	201.9	201.6
800	273.5	273.3	158.1	157.7	148.7	149.2	57.7	57.8	196.6	196.2
1,000	266.8	266.0	153.6	154.0	145.6	146.1	56.0	56.0	191.2	191.3

Table 6 MnO: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{12}		C_{44}		C_S		B_S	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	223.5	223.5	111.8	111.8	78.1	78.1	55.9	55.9	149.0	149.0
350	220.6	220.4	111.8	111.8	77.7	78.1	54.4	54.3	148.1	148.0
400	217.8	217.2	111.8	111.8	77.3	77.8	53.0	52.7	147.1	146.9
450	214.9	214.1	111.8	111.7	76.8	77.3	51.6	51.2	146.1	145.8
500	212.1	210.9	111.8	111.7	76.0	76.5	50.2	49.6	145.2	144.8

Table 7 NaCl: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{12}		C_{44}		C_S		B_S	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	49.5	49.5	13.2	13.2	12.79	12.79	18.1	18.1	25.3	25.3
350	47.7	47.6	13.20	13.3	12.61	12.62	17.3	17.1	24.7	24.8
450	44.0	44.1	13.19	13.5	12.26	12.26	5.4	15.3	23.5	23.7
550	40.4	40.5	13.18	13.5	11.91	11.90	13.6	13.5	22.3	22.5
650	36.7	37.0	13.17	13.1	11.55	11.52	11.8	11.9	21.0	21.1
750	33.2	33.7	13.16	12.9	11.20	11.10	10.0	10.4	19.8	19.8

Table 8 Olivine $Fe_{90}Fa_{10}$: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{22}		C_{33}		C_{44}		C_{55}		C_{66}		C_{23}		C_{31}		C_{12}	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	320.6	320.6	197.1	197.1	234.2	234.2	63.7	63.7	77.6	77.6	78.3	78.3	74.8	74.8	71.2	71.2	69.8	69.8
500	312.4	313.0	190.8	190.9	227.1	227.6	61.2	61.0	75.0	74.9	75.1	74.9	73.3	73.7	69.2	69.3	67.5	67.4
700	304.2	305.0	184.5	184.6	220.0	220.6	58.7	58.4	72.5	72.3	71.9	71.7	71.9	72.3	67.1	67.2	65.2	65.0
900	296.0	297.0	178.2	178.3	212.9	214.3	56.2	55.9	69.9	69.9	68.7	68.5	70.4	71.2	65.1	66.0	62.9	62.8
1,100	287.8	289.0	171.9	172.3	205.8	206.6	53.7	53.4	67.4	67.1	65.6	65.5	69.0	69.4	63.0	63.4	60.6	60.5
1,300	279.6	280.9	165.7	166.1	198.7	199.3	51.2	51.0	64.8	64.5	62.4	62.5	67.5	67.8	61.0	61.4	58.3	58.2
1,500	271.4	272.0	159.4	159.8	191.7	192.1	48.7	48.5	62.7	62.2	59.2	59.5	66.1	66.4	58.9	59.8	56.0	56.2

Table 9 Fe_2SiO_4: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{22}		C_{33}		C_{44}		C_{55}		C_{66}		C_{23}		C_{31}		C_{12}	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	266.9	266.9	173.5	173.5	239.1	239.1	32.4	32.4	46.7	46.7	57.3	57.3	97.9	97.9	98.7	98.7	95.1	95.1
400	262.9	262.2	169.9	170.1	234.4	234.7	32.2	31.7	46.4	46.0	55.7	55.3	97.2	97.4	97.8	97.7	93.3	93.4
500	259.0	258.8	166.3	166.6	229.7	229.9	32.0	31.4	46.2	45.8	54.1	53.7	96.5	96.8	96.9	97.0	91.5	91.9
600	255.0	255.0	162.6	162.8	225.1	225.1	31.8	31.5	45.9	45.6	52.5	52.3	95.9	96.0	96.1	96.1	89.7	90.0
700	251.0	251.0	159.0	159.0	220.4	220.5	31.9	31.6	45.6	45.5	50.9	51.0	95.2	94.8	95.2	94.9	88.0	87.7

Table 10 Mn_2SiO_4: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{22}		C_{33}		C_{44}		C_{55}		C_{66}		C_{23}		C_{31}		C_{12}	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	258.3	258.3	165.5	165.5	206.7	206.7	45.3	45.3	55.6	55.6	57.8	57.8	91.7	91.7	95.2	95.2	87.1	87.1
400	254.8	254.8	162.8	162.7	203.8	203.9	44.4	44.4	54.7	54.4	56.4	56.4	90.6	90.6	93.8	93.8	85.6	85.5
500	251.4	251.3	160.1	159.8	201.0	201.0	43.6	43.5	53.8	52.3	55.0	53.8	89.5	93.4	92.4	93.2	84.1	85.1
600	247.9	247.8	157.4	157.0	198.1	198.2	42.7	42.5	52.9	52.0	53.6	53.7	88.4	88.3	91.1	90.8	82.6	82.2
700	244.5	244.3	154.7	154.2	195.3	195.3	41.8	41.5	52.0	51.8	52.2	52.4	87.2	87.2	89.7	89.4	81.1	80.6

Table 11 Co_2SiO_4: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{22}		C_{33}		C_{44}		C_{55}		C_{66}		C_{23}		C_{31}		C_{12}	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	307.7	30707	194.7	194.7	234.1	234.1	46.7	46.7	63.9	63.9	64.8	64.8	103.2	103.2	105.0	105.0	101.6	101.6
400	304.3	304.0	192.4	192.6	230.9	230.7	46.1	46.2	62.9	62.9	63.7	63.8	101.7	101.8	103.5	103.6	99.8	99.8
500	300.9	301.1	190.2	190.5	227.6	227.4	45.6	45.7	61.8	61.9	62.5	62.8	100.2	100.5	102.1	102.3	98.0	97.9
600	297.4	297.8	187.9	188.6	224.4	224.0	45.0	45.2	60.8	60.8	61.4	61.8	98.7	99.1	100.6	100.9	96.3	96.1
700	294.0	294.5	185.7	186.2	221.1	220.6	44.4	44.7	59.7	59.8	60.3	60.8	97.2	97.8	99.2	99.6	94.5	94.3

Table 12 Al_2O_3: calculated values of elastic moduli (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic conditions

T (K)	C_{11}		C_{33}		C_{44}		C_{12}		C_{13}		C_{14}	
	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]	Eq. 12	[2]
300	497.2	497.2	500.8	500.8	146.7	146.7	162.8	162.8	116.0	116.0	–21.9	–21.9
600	483.2	486.0	486.3	489.2	139.3	139.2	162.4	163.1	112.7	113.0	–22.5	–23.3
900	469.2	472.3	471.8	476.0	131.9	131.2	161.9	162.4	109.4	109.6	–23.1	–23.9
1,200	455.2	457.3	457.3	461.1	124.6	123.2	161.5	160.7	106.2	105.4	–23.7	–24.3
1,500	441.2	442.2	442.8	446.4	117.2	115.1	161.0	159.4	102.9	101.6	–24.2	–24.5
1,800	427.2	427.2	428.4	432.5	109.9	107.4	160.6	158.0	99.6	99.1	–24.8	–24.5

of these results reveals the validity of the exponential dependence as represented by Eq. 11 for different elastic moduli. It can be concluded that the present assumption that α depends quadratically on temperature is more logical and physically realistic.

Because of the difference between δ_{S_0} and δ_{T_0}, B_T and B_S show very different temperature dependences. For the case of NaCl, the calculated values of B_T at different temperatures are reported in Table 2, and the calculated values of B_S are reported in Table 10. The variation of B_T with temperature is found to be large as compared with B_S.

In summary, we have presented a simple method in order to determine the temperature dependence of the elastic properties of solids. Ten solids are presented as examples because the required experimental data are readily available here, permitting direct comparisons. The simplicity of the method lies in the fact that it does not involve the use of a two- or three-body potential, thus permitting investigations of the elastic properties of more complex materials at higher temperature where experimental data are not available.

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