
Elastic Constants for Various Classes of Solids at High Temperature

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In the present communication, a new relationship for the temperature dependences of elastic constants are developed using a new expression for the temperature dependence of bulk modulus and the formulation derived from Tallon's model. The proposed relationship is applied to study elastic constants of NaCl, KCl, CaF₂, MgO, CaO, and Mg₂SiO₄. The result obtained for second-order elastic constants are found to compare well with the experimental data.

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1. Introduction

The knowledge of elastic constants is essential to interpret the thermodynamic and elastic dimensions of solids at high temperatures. The elasticity offers more information than the volume in interpreting the temperature dependence of equation of state because the compressibility is defined by the derivative of volume. The elastic constants also provide a ground for examining of Earth's deep interior [1]. The behaviors of elastic constants under the influence of high temperature have attracted the attention of experimental [2–4] as well as theoretical workers [5–8]. 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 lot of computational work in addition to various approximations. Thus, it may be useful to propose a simple and straightforward method for predicting high-temperature elastic constants, which is the purpose of the present paper.

In this paper, first we develop a new expression for the temperature dependence of bulk modulus by using fundamental thermodynamic relations simultaneously assuming that the volume thermal expansion coefficient is a quadratic

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function of temperature. By combining the new expression with the formulation derived from Tallon's model [9], then we calculate the temperature dependences of elastic constants for NaCl, KCl, CaF₂, MgO, CaO, and Mg₂SiO₄. The results are found to yield a close agreement with the available experimental data, which in turn, reveals the validity of the present work.

2. A new expression for the temperature dependence of bulk modulus

The Anderson–Grüneisen parameter, which plays an important role in understanding the anharmonic properties of ionic solids, is defined as follows [10]:

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

where α and B_T are the coefficient of volume thermal expansion and isothermal bulk modulus, respectively.

They are defined as

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

and

$$B_T = \frac{1}{V} \left(\frac{\partial P}{\partial V} \right)_T. \quad (3)$$

A method to estimate the temperature dependence of the bulk modulus has been developed with the approximation that α depends linearly on temperature [11]. But we find that, in the case of NaCl whose experimental results had been reported, the values of B_T calculated in Ref. [11] is adequate for small expansions. The percentage differences increase with increasing temperature and become 9.75% at 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 comparing and analyzing some experimental data, this paper puts forward that α depends quadratically on temperature, which can be written as follows:

$$\alpha = \alpha_0 + \alpha'_0(T - T_0) + \frac{\alpha''_0}{2}(T - T_0)^2, \quad (4)$$

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 $T = T_0 = 300$ K. If one assumes that the product αB_T remains constant [12], then we get from Eq. (1) the following approximate formulation:

$$\delta_T = \frac{1}{\alpha^2} \left(\frac{\partial \alpha}{\partial T} \right)_P. \quad (5)$$

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

$$\alpha'_0 = \left(\frac{\partial \alpha}{\partial T} \right)_P = \delta_T \alpha_0^2 \quad (6)$$

and

$$\alpha_0'' = \left(\frac{\partial^2 \alpha}{\partial T^2} \right)_P = 2\delta_{T_0}^2 \alpha_0^3, \quad (7)$$

where δ_{T_0} is the value of δ_T at T_0 and at atmospheric pressure, i.e. at $P = 0$. Therefore Eq. (4) can be rewritten as follows:

$$\alpha = \alpha_0 + \delta_{T_0} \alpha_0^2 (T - T_0) + \delta_{T_0}^2 \alpha_0^3 (T - T_0)^2. \quad (8)$$

Substituting the value of α from Eq. (8) in Eq. (1), we get

$$\frac{dB_T}{B_T} = -\delta_{T_0} [\alpha_0 + \delta_{T_0} \alpha_0^2 (T - T_0) + \delta_{T_0}^2 \alpha_0^3 (T - T_0)^2] dT. \quad (9)$$

Integrating Eq. (9), we finally get the following expression for $B_T(T)$:

$$\frac{B_T}{B_{T_0}} = \exp \left(-\delta_{T_0} \alpha_0 (T - T_0) \left(1 + \frac{\delta_{T_0} \alpha_0 (T - T_0)}{2} + \frac{\delta_{T_0}^2 \alpha_0^2 (T - T_0)^2}{3} \right) \right), \quad (10)$$

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

3. The expressions for the temperature dependence of elastic constants

Grover et al. [13] used a non-standard definition of δ_T and recalled it the parameter g as given below

$$g = -\frac{V_0}{B_T} \left(\frac{\partial B_T}{\partial V} \right)_P, \quad (11)$$

where V_0 is the value of V at $P = 0$. Equation (11) when generalized reads as follows:

$$g_m = -\frac{V_0}{M} \left(\frac{\partial M}{\partial V} \right)_P, \quad (12)$$

where M represents any of the elastic moduli, such as C_{11} , C_{12} , C_{44} , $(C_{11} - C_{12})/2$ or B_T . Tallon [9] has expressed Eq. (12) as follows:

$$\frac{M}{M_0} = \exp \left(-g_m \left(\frac{V}{V_0} - 1 \right) \right). \quad (13)$$

Equation (13) may be used to determine the temperature dependence of elastic constants. Following the method of generalization as used by Tallon [9] to get Eq. (13), we can generalize Eq. (10) as follows:

$$\frac{M}{M_0} = \exp \left(-\delta_{M_0} \alpha_0 (T - T_0) \left(1 + \frac{\delta_{M_0} \alpha_0 (T - T_0)}{2} + \frac{\delta_{M_0}^2 \alpha_0^2 (T - T_0)^2}{3} \right) \right). \quad (14)$$

In Eq. (14), δ_{M_0} should vary according to the elastic moduli selected. On the basis of Eq. (14), the relevant expression for elastic constants may be written collectively as follows:

$$\frac{C_{ij}}{C_{ij_0}} = \exp \left(-\delta_{ij_0} \alpha_0 (T - T_0) \left(1 + \frac{\delta_{ij_0} \alpha_0 (T - T_0)}{2} + \frac{\delta_{ij_0}^2 \alpha_0^2 (T - T_0)^2}{3} \right) \right). \quad (15)$$

Here δ_{ij_0} is given by Eq. (1) as defined by Kumar and Bedi [14].

4. Results and discussions

Equation (10), obtained by the authors, is used to compute the values of B_T at different T , using the input data [2, 5, 15] given in Table I. The results obtained from Ref. [11] are also included in Table II for the sake of comparison. It is found that Eq. (10) improves the results as compared with Ref. [11]. Thus, Eq. (10) proposed by the authors seems to be suitable for the temperature dependence of bulk modulus. This encouraged the authors to extend Eq. (10) for the study of the variation of elastic moduli. Equation (10) may be generalized in the form of Eq. (14). Equation (14) may be written for the second-order elastic constants (SOEC) in

TABLE I

Values of input parameters [2, 5, 15]. α_0 in $[10^{-6} \text{ K}^{-1}]$.

	NaCl	KCl	CaF ₂	MgO	CaO	MgSiO ₄
α_0	118	110	56	31.2	30.4	27.2
δ_{110}	6.27	7.48	3.43	6.27	7.3	4.06
δ_{120}	0.051	-3.31	4.61	-2.49	-2.0	6.00
δ_{440}	2.34	3.05	6.50	2.57	2.9	7.50
δ_{220}	-	-	-	-	-	5.07
δ_{230}	-	-	-	-	-	3.20
δ_{310}	-	-	-	-	-	5.10
δ_{330}	-	-	-	-	-	4.50
δ_{550}	-	-	-	-	-	6.60
δ_{660}	-	-	-	-	-	7.50

TABLE II

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 (1050 K)	107.4	117.5	119.0
Percentage deviation at T_m	9.75	1.26	-

TABLE III

NaCl: Calculated values of C_{11} , C_{12} , and C_{44} (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic condition.

T [K]	C_{11}		C_{12}		C_{44}	
	Eq. (15)	[2]	Eq. (15)	[2]	Eq. (15)	[2]
300	49.5	49.5	13.2	13.2	12.79	12.79
350	47.7	47.6	13.20	13.3	12.61	12.62
400	45.8	45.8	13.19	13.4	12.44	12.43
450	44.0	44.1	13.19	13.5	12.26	12.26
500	42.2	42.4	13.18	13.6	12.08	12.09
550	40.4	40.5	13.18	13.5	11.91	11.90
600	38.5	38.7	13.18	13.2	11.73	11.71
650	36.7	37.0	13.17	13.1	11.55	11.52
700	34.9	35.4	13.17	13.1	11.38	11.31
750	33.2	33.7	13.16	12.9	11.20	11.10

TABLE IV

KCl: Calculated values of C_{11} , C_{12} , and C_{44} (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic condition.

T [K]	C_{11}		C_{12}		C_{44}	
	Eq. (15)	[2]	Eq. (15)	[2]	Eq. (15)	[2]
300	40.1	40.1	6.6	6.6	6.35	6.35
350	38.5	38.4	6.7	6.8	6.24	6.28
400	36.8	36.9	6.8	7.0	6.14	6.21
450	35.2	35.4	7.0	7.1	6.03	6.15
500	33.5	33.8	7.1	7.2	5.92	6.11
550	31.9	32.3	7.2	7.3	5.82	6.05
600	30.2	31.1	7.3	7.5	5.71	5.96
650	28.6	29.7	7.4	7.7	5.60	5.87
700	27.0	28.2	7.6	7.7	5.50	5.79
750	25.4	26.6	7.7	7.7	5.39	5.69
800	23.9	25.2	7.8	7.8	5.29	5.57
850	22.3	23.5	7.9	7.7	5.18	5.57

the form of Eq. (15) which is used to compute the temperature dependence of SOEC of NaCl, KCl, CaF₂, MgO, CaO, and Mg₂SiO₄. The results thus obtained are given in Tables III–VIII along with the experimental data ([2, 5, 15] and [16]).

TABLE V

CaF₂: Calculated values of C_{11} , C_{12} , and C_{44} (in GPa) at different temperatures along with the experimental data [16] obtained under adiabatic condition.

T [K]	C_{11}		C_{12}		C_{44}	
	Eq. (15)	[16]	Eq. (15)	[16]	Eq. (15)	[16]
300	165.5	165.5	40.7	40.7	33.5	33.5
400	162.3	162.6	39.6	39.3	32.3	32.6
500	159.1	160.6	38.6	38.6	31.1	32.0
600	156.0	158.0	37.5	38.2	29.8	31.3
700	152.8	154.6	36.5	37.5	28.6	30.6
800	149.6	150.0	35.4	36.8	27.4	30.0
900	146.4	146.6	34.4	35.7	26.2	28.6
1000	143.3	142.0	33.4	34.3	25.0	27.0
1100	140.1	138.0	32.3	32.9	23.8	26.2
1200	136.9	132.0	31.3	32.2	22.6	25.3

TABLE VI

MgO: Calculated values of C_{11} , C_{12} , and C_{44} (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic condition.

T [K]	C_{11}		C_{12}		C_{44}	
	Eq. (15)	[2]	Eq. (15)	[2]	Eq. (15)	[2]
300	298.96	298.96	96.42	96.42	157.13	157.13
400	293.11	292.94	97.17	97.17	155.87	155.78
600	281.41	280.62	98.67	98.00	153.35	152.84
800	269.72	268.22	100.17	98.54	150.83	149.68
1000	258.05	255.74	101.66	98.74	148.31	146.52
1200	246.39	243.32	103.16	98.38	145.79	143.06
1400	234.78	230.96	104.16	97.56	143.27	139.54
1600	223.22	219.04	106.16	96.44	140.76	136.24
1800	211.75	208.18	107.66	95.02	138.24	133.12

In the case of NaCl, KCl, CaF₂, MgO, and CaO, there are only three SOEC viz. C_{11} , C_{12} , C_{44} . The results obtained for the elastic constants for these five solids under study present reasonably good agreement with the available experimental data ([2, 5] and [15]). And from the above, the variation of C_{11} with temperature is found to be larger as compared with C_{12} and C_{44} . The constant C_{11} represents elasticity in length. A longitudinal strain produces a change in volume without a change in shape. The volume change is highly related to the

TABLE VII

CaO: Calculated values of C_{11} , C_{12} , and C_{44} (in GPa) at different temperatures along with the experimental data [2] obtained under adiabatic condition.

T [K]	C_{11}		C_{12}		C_{44}	
	Eq. (15)	[2]	Eq. (15)	[2]	Eq. (15)	[2]
300	220.5	220.5	57.67	57.67	80.03	80.03
400	215.6	215.7	58.02	57.96	79.32	79.35
500	210.7	210.7	58.37	58.23	78.62	78.70
600	205.8	205.9	58.72	58.44	77.91	77.94
700	200.9	201.2	59.07	58.66	77.20	77.18
800	196.0	196.6	59.42	58.81	76.50	76.46
900	191.1	192.0	59.77	58.98	75.79	75.72
1000	186.2	187.2	60.12	58.98	75.09	74.92
1100	181.3	182.7	60.47	58.96	74.38	74.17
1200	176.5	178.1	60.82	58.99	73.67	73.48

TABLE VIII

MgSiO₄: Calculated values of elastic constants (in GPa) at different temperatures (top) along with the experimental data [2] (bottom) obtained under adiabatic condition. The first value of C_{ij} comes from Eq. (15), the second one from [2].

T [K]	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{23}	C_{31}	C_{12}
300	330.0	200.0	236.0	67.2	81.5	81.2	71.2	68.0	66.2
	330.0	200.0	236.0	67.2	81.5	81.2	71.2	68.0	66.2
500	322.7	194.5	230.2	64.5	78.6	77.9	70.0	66.1	64.0
	322.4	194.2	230.1	64.4	78.7	78.0	71.1	66.1	64.0
700	315.4	189.0	224.4	61.7	75.6	74.6	68.7	64.2	61.9
	314.5	188.0	223.6	61.6	75.8	74.6	69.7	64.3	61.8
900	308.1	183.5	218.7	59.0	72.7	71.3	67.5	62.3	59.7
	306.3	181.5	216.9	58.8	72.8	71.3	68.3	62.5	59.4
1100	300.9	177.9	212.9	56.2	69.8	68.0	66.2	60.5	57.6
	297.4	175.1	209.8	56.1	69.9	67.9	67.2	60.5	57.3
1300	293.6	172.4	207.1	53.5	66.9	64.7	65.0	58.6	55.4
	288.3	168.7	202.7	53.3	66.9	64.6	66.0	58.5	55.3
1500	286.3	166.9	201.4	50.8	64.0	61.4	63.8	56.7	53.3
	279.1	162.2	195.5	50.6	64.0	61.4	64.6	56.7	53.2
1700	279.0	161.5	195.6	48.1	61.0	58.3	62.5	54.8	51.1
	269.8	155.6	188.2	48.0	61.0	58.4	63.3	54.9	51.0

temperature and thus produces a large change in C_{11} . On the other hand, the constants C_{12} and C_{44} are related to the elasticity in shape which is shear constant. A transverse strain or shearing causes a change in shape without a change in volume. Thus C_{12} and C_{44} are less sensitive of temperature as compared with C_{11} .

Equation (15) has also been extended to calculate the SOEC of more complicated minerals, viz. Mg_2SiO_4 . For Mg_2SiO_4 , there are nine SOEC, the calculated values of SOEC are also found to be in very good agreement with the experimental data [2]. The maximum deviation found for C_{33} at highest temperature (1700 K) is 3.93%.

To summarize, we have thus presented a simple and straightforward method to study the elastic properties of solids under the varying conditions of temperatures. The results obtained are encouraging and demonstrate that the present method is reasonable. Due to the simplicity of the method, it can be extended to more complex solids like minerals at higher temperature.

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elastic constants of diamond with temperature. Several types of covalent atoms have been parametrized. within the second-generation REBO formalism. A quantitative dependence of elastic constants on temperature, along with the widespread use of the Brenner potential, a parametrization for silicon (2B-Si) within the second-generation REBO formalism has been developed. The pa For the remaining solid Si structures, bond energies and force constants were calculated at each structure's minimum-energy bond length using Eq. (1) or its second derivative, respectively. There are three general classes of material model for solids. 1. The material is close to ideally elastic. i.e. (i) when deformed at constant temperature or adiabatically, stress is a function only of current strain and independent of history or rate of loading, (ii) the behavior is reversible: no net work is done on the solid when subjected to a closed cycle of strain under adiabatic or isothermal conditions. Isotropic solids are of particular interest. These are materials that are unchanged by all proper orthogonal transformations of the reference configuration. In some cases this is quite simple (the incompressible neo-Hookean material only has 1 constant!); for models like the generalized polynomial or Ogden's it is considerably more involved. Conceptually, however, the procedure is straightforward. The knowledge of elastic constants is essential to interpret the thermodynamic and elastic dimensions of solids at high temperatures. The elasticity offers more information than the volume in interpreting the temperature dependence of equation of state because the compressibility is dened by the derivative of volume. The elastic constants also provide a ground for examining of Earth's deep interior [1]. The behaviors of elastic constants under the influence of high temperature have attracted the attention of experimental [2-4] as well as theoretical workers [5-8]. It has been...