

Research Article

Temperature Dependence of Elastic Constants of Alkaline Earth Oxides

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The elastic properties of alkaline earth oxides (AEOs) under high temperature are discussed within the framework of many body Lundqvist potential incorporating the contribution of thermal phonon pressure. The short-range repulsive interaction is taken up to the second nearest neighbors. The derived expressions are used to compute the values of second-order elastic constants (SOECs) and bulk modulus of alkaline earth oxides at different temperatures (300° K–2000° K). The results are found to be satisfactory and are in agreement with available experimental and the theoretical results.

1. Introduction

The general theory for the thermoelastic behaviour of ionic solid was first of all given by Wallace [1]. Srivastava [2, 3] and Varshney [4] have applied it to the solids crystallizing in NaCl and CsCl structure. Kumar and coworker [5–7] have analyzed the variation of elastic constant with temperature for MgO and CaO using different approaches modifying the Suzuki relation of equation of state [8]. However, their results [5–7] are better than Suzuki's results but are much different from the experimental results. Any equation of state contains the bulk modulus and its derivatives as dependent parameter. The results obtained by Kumar and coworkers [5–7] show the worse agreement between the computed values of bulk modulus at different temperatures with their experimental results in case of MgO and CaO. This clearly indicates that modification improves some values of the elastic constants at different temperatures but shows poor agreement of bulk modulus at different temperature. It may be due to the reason that they have not considered the higher order terms that is, anharmonic terms, in the expansion of the logarithmic series of volume change. But the elastic properties are directly related to the lattice potential which consists of the various interaction systems.

In the present study, we have used many body Lundqvist potentials [13–15] incorporating thermal phonon pressure to study the second-order elastic constant of all alkaline

earth oxides solid, that is, MgO, CaO, SrO, and BaO solid at different temperatures (up to 2000° K). This potential has been recently used [11, 16, 17] to explain the elastic properties of alkaline earth oxides (AEOs) and rare gas solids (RGs) at different pressures. The potential has been suitably modify to take into consideration the changes in the lattice parameter due to the increase in temperature. Now we have derived the relation of second-order elastic constants by modifying the lattice parameter. The results predicted by the present theory are discussed and compared with available experimental and others theoretical results.

2. Theory

The total lattice energy of diatomic solid [14] is regarded as

$$\Phi(r) = \frac{e^2}{2} \sum_k \sum_{l'k'} \frac{\in(k) \in(k')}{r(l',kk')} + e^2 \sum_k \sum_{NN} V' \{r(l',kk')\} + e^2 \sum_k \sum_{l'k'} \sum_{l''k''} f_{k''} \{r(l'',kk'')\} \frac{\in(k')}{r(l',kk')}, \quad (1)$$

where $\in(k)$ is the valency of k type ion, \in the magnitude of $\in(k)$, and $r(l',kk')$ the interionic separation between ion $\binom{0}{k}$ at origin to ion $\binom{l'}{k'}$. The first term represents Coulomb energy, the second the overlap repulsive energy coupling the neighbours and the third term the three body

TABLE 1: Values of input data at room temperature; a , r_+ , r_- , and ρ are (all in Å°), (in 10^{-12} erg), $\beta(10^{-5} \text{K}^{-1})$ and elastic constants and bulk modulus (in GPa).

Solids	C_{11}	C_{12}	C_{44}	a	r_+	r_-	ρ	b	β	K
MgO	298.96 ^(a)	96.42 ^(a)	157.13 ^(a)	2.125 ^(c)	0.78 ^(d)	1.32 ^(d)	0.347 ^(d)	2.003 ^(d)	3.12 ^(d)	159.67 ^(a)
CaO	220.53 ^(a)	57.67 ^(a)	80.03 ^(a)	2.42 ^(c)	1.06 ^(d)	1.32 ^(d)	0.386 ^(d)	2.010 ^(d)	3.04 ^(d)	111.96 ^(a)
SrO	173 ^(b)	45 ^(b)	56 ^(b)	2.598 ^(c)	1.27 ^(d)	1.32 ^(d)	0.390 ^(d)	1.900 ^(d)	4.2 ^(d)	91 ^(b)
BaO	121 ^(c)	50 ^(c)	38 ^(c)	2.776 ^(c)	1.74 ^(d)	1.32 ^(d)	0.415 ^(d)	1.747 ^(d)	3.8 ^(d)	69 ^(c)

^(a)Ref[9], ^(b)Ref[10], ^(c)Ref[11], ^(d)Ref[12].

TABLE 2

(a) Calculated values of C_{11} (GPa) for MgO at different temperatures T (K).

T	Pre	Su [7]	Ku [7]	Exp.[9]
300	299	298.96	298.96	298.96
400	293	293.08	293.1	292.94
500	287.1	287.17	287.24	
600	281.2	281.22	281.38	280.62
700	275.4	275.22	275.55	
800	269.7	269.18	269.76	268.22
900	264	263.09	264.02	
1000	258.4	256.97	258.34	255.74
1100	252.8	250.8	252.72	
1200	247.3	244.59	247.18	243.22
1300	241.8	238.34	241.72	
1400	236.3	232.05	236.36	230.96
1500	231	225.71	231.08	
1600	225.6	219.34	225.91	219.04
1700	220.3	212.91	220.84	
1800	215.1	206.45	215.88	208
1900	209.9	199.94	210.97	
2000	204.7	193.39	206.22	

(b) Calculated values of C_{12} (Gpa) for MgO at different temperatures T (K).

T	Pre	Su [7]	Ku [7]	Exp.[9]
300	96.42	96.42	96.42	96.42
400	95.84	97.17	97.17	97.14
500	95.28	97.92	97.92	
600	94.74	98.68	98.67	98
700	94.22	99.44	99.43	
800	93.72	100.2	100.18	98.54
900	93.22	100.97	100.93	
1000	92.75	101.73	101.7	98.74
1100	92.29	102.51	102.46	
1200	91.85	103.28	103.22	98.38
1300	91.42	104.06	103.98	
1400	91.01	104.84	104.74	97.56
1500	90.62	105.62	105.5	
1600	90.24	106.4	106.26	96.44
1700	89.87	107.19	107.03	
1800	89.52	107.98	107.79	95.02
1900	89.18	108.77	108.56	
2000	88.85	109.57	109.32	

(c) Calculated values of C_{44} (GPa) for MgO at different temperatures T (K)

T	Pre	Su [7]	Ku [7]	Exp.[9]
300	157.1	157.13	157.13	157.13
400	156.3	155.86	155.86	155.78
500	155.5	154.58	154.6	
600	154.8	153.3	153.33	152.84
700	154.1	152.01	152.05	
800	153.4	150.69	150.78	149.68
900	152.7	149.37	149.5	
1000	152	148.04	148.23	146.52
1100	151.4	146.7	146.95	
1200	150.8	145.34	145.68	143.06
1300	150.3	143.98	144.41	
1400	149.7	142.61	143.14	139.54
1500	149.2	141.22	141.88	
1600	148.7	139.82	140.62	136.24
1700	148.3	138.42	139.37	
1800	147.8	137	138.12	133.12
1900	147.4	135.57	136.88	
2000	147	134.13	135.64	

(d) Calculated values of K (GPa) for MgO at different temperatures T (K).

T	Pre	Su [7]	Ku [7]	Exp.[9]
300	163.9	163.93	163.9	163.9
400	161.6	162.47	161.18	162.3
500	159.2	161.01	158.47	
600	156.9	159.53	155.75	158.9
700	154.6	158.03	153.04	
800	152.4	156.53	150.34	155.1
900	150.2	155.01	147.65	
1000	148	153.48	144.99	151.1
1100	145.8	151.94	142.34	
1200	143.7	150.38	139.73	146.7
1300	141.5	148.82	137.14	
1400	139.5	147.24	134.59	142
1500	137.4	145.65	132.07	
1600	135.4	144.05	129.58	137.3
1700	133.4	142.43	127.14	
1800	131.4	140.8	124.73	132.6
1900	129.4	139.16	122.37	
2000	127.5	137.51	120.05	

potential. The function f is related to the overlap integrals of free-ion one electron wave functions and is assumed significant only for nearest neighbours and is related to overlap integrals reported by Hafmeister and Flygare [18]. However, in the present study, we have chosen this function f and its derivatives as disposable parameters at $r = a$, the nearest-neighbour distance. On simplification, the above

lattice energy per unit cell $\phi(r)$ for alkaline earth oxide solids can be expressed as

$$\Phi(r) = \frac{\alpha_m (\epsilon + 12f(r)) e^2}{r} + N\phi_1(r) + N'\phi_2(r), \quad (2)$$

where $\alpha_m (= 1.7476)$ is the Madelung constant for NaCl structure. N and N' are the numbers of the nearest and next

TABLE 3
(a) Calculated values of C_{11} (GPa) for CaO at different temperatures T (K).

T	Pre	Su [7]	Ku [7]	Exp.[9]
300	221	220.53	220.53	220.5
400	216	220.03	215.62	215.7
500	212	219.54	210.72	210.7
600	208	219.03	205.82	205.9
700	204	218.51	200.96	201.2
800	200	217.99	196.14	196.6
900	196	217.46	191.37	192
1000	192	216.93	186.67	187.2
1100	188	216.38	182.03	182.7
1200	184	215.83	177.47	178.1
1300	180	215.27	172.99	
1400	176	214.71	168.61	
1500	173	214.14	164.32	
1600	169	213.56	160.13	
1700	165	212.97	156.03	
1800	161	212.36	152.04	
1900	158	211.79	148.15	
2000	154	211.18	144.37	

(b) Calculated values of C_{12} (GPa) for CaO at different temperatures T (K).

T	Pre	Su [7]	Ku [7]	Exp.[9]
300	57.67	57.6	57.6	57.67
400	57.39	57.63	57.95	57.96
500	57.13	57.66	58.3	58.23
600	56.87	57.7	58.65	58.44
700	56.63	57.73	59	58.66
800	56.39	57.76	59.35	58.81
900	56.17	57.79	59.71	58.98
1000	55.95	57.82	60.06	58.98
1100	55.75	57.85	60.41	58.96
1200	55.55	57.88	60.77	58.99
1300	55.36	57.9	61.12	
1400	55.18	57.93	61.48	
1500	55.01	57.96	61.83	
1600	54.84	57.98	62.19	
1700	54.69	58	62.55	
1800	54.54	58.03	62.9	
1900	54.4	58.05	63.26	
2000	54.27	58.07	63.62	

(c) Calculated values of C_{44} (GPa) for CaO at different temperatures T (K).

T	Pre	Su [7]	Ku [7]	Exp.[9]
300	80.03	80.03	80.03	80.03
400	79.83	79.96	79.33	79.35
500	79.66	79.88	78.62	78.7

(c) Continued.

T	Pre	Su [7]	Ku [7]	Exp.[9]
600	79.49	79.81	77.92	77.94
700	79.34	79.73	77.21	77.18
800	79.2	79.65	76.5	76.46
900	79.08	79.58	75.79	75.72
1000	78.97	79.49	75.09	74.92
1100	78.87	79.41	74.38	74.17
1200	78.79	79.32	73.68	73.48
1300	78.71	79.24	72.98	
1400	78.65	79.14	72.28	
1500	78.6	79.05	71.58	
1600	78.56	78.96	70.89	
1700	78.54	78.86	70.19	
1800	78.52	78.76	69.51	
1900	78.52	78.66	68.82	
2000	78.52	78.56	68.15	

(d) Calculated values of K (GPa) for CaO at different temperatures T (K).

T	Pre	Su [7]	Ku [7]	Exp.[9]
300	112	111.91	111.96	111.96
400	110.4	111.77	110.05	110.53
500	108.8	111.62	108.14	109.06
600	107.3	111.47	106.23	107.59
700	105.7	111.32	104.32	106.18
800	104.2	111.17	102.43	104.73
900	102.7	111.02	100.54	
1000	101.3	110.86	98.67	
1100	99.82	110.69	96.82	
1200	98.38	110.53	94.98	
1300	96.97	110.36	93.17	
1400	95.57	110.19	91.38	
1500	94.19	110.02	89.62	
1600	92.83	109.84	87.88	
1700	91.48	109.66	86.17	
1800	90.15	109.48	84.49	
1900	88.84	109.29	82.84	
2000	87.54	109.11	81.22	

to nearest neighbours. $\phi_1(r)$ and $\phi_2(r)$ are the short range potentials between nearest neighbours and next nearest neighbours related to Lundqvist potential as follows:

$$\begin{aligned} \phi'_1(r) &= \phi_1(r) + \frac{\alpha_m}{a} \in f(r), \\ \phi'_2(r) &= \phi_2(r) \\ &= \frac{1}{2}b \left[\beta_{++} \exp\left(\frac{2r_+}{\rho}\right) + \beta_{--} \exp\left(\frac{2r_-}{\rho}\right) \right] \exp\left(-\frac{\sqrt{2}r}{\rho}\right), \end{aligned} \quad (3)$$

where b and ρ are the Born repulsive parameters. r_+ and r_- are the characteristic length for the positive and negative ions. β_{ij} are Pauling coefficients [19] defined as follows:

$$\beta_{ij} = 1 + \left(\frac{\in_i}{p_i}\right) + \left(\frac{\in_j}{p_j}\right), \quad (4)$$

where \in_i and \in_j are the valencies of two ions. p_i and p_j are the number of outermost electrons in ions i and j .

Considering that the vibrational energy of the solid is a purely temperature dependent function as

$$\left(\frac{d\Phi}{dr}\right)_{r=a} = -P + T\beta K \quad (5)$$

TABLE 4: Calculated values of C_{11} , C_{12} , C_{44} , and K (GPa) for SrO at different temperatures T (K).

T	C_{11}	C_{12}	C_{44}	K
300	173	45	56	87.67
400	168.36	44.73	55.94	85.94
500	163.78	44.47	55.92	84.25
600	159.27	44.24	55.91	82.58
700	154.81	44.01	55.9	80.95
800	150.41	43.8	55.92	79.34
900	146.06	43.6	55.96	77.76
1000	141.77	43.42	56.01	76.2
1100	137.54	43.25	56.08	74.68
1200	133.35	43.09	56.17	73.17
1300	129.21	42.94	56.27	71.7
1400	125.13	42.8	56.38	70.25
1500	121.08	42.68	56.51	68.81
1600	117.09	42.57	56.65	67.41
1700	113.15	42.47	56.81	66.03
1800	109.24	42.38	56.98	64.67
1900	105.38	42.31	57.16	63.33
2000	101.56	42.24	57.36	62.01

and using the above lattice potential functions (1) and (3), the expressions for second-order elastic constant at any temperature T for alkaline earth oxides are derived as

$$\begin{aligned}
C_{11} &= -4.388T\beta K_T \\
&+ \frac{e^2}{4\eta^4} \left\{ A_1 + \frac{A_2}{2} + 4.388B_1 + 4.888B_2 + 9.3204 \in \left(a \frac{\partial f}{\partial r} \right) \right\}, \\
C_{12} &= 1.194T\beta K_T \\
&+ \frac{e^2}{4\eta^4} \left\{ \frac{A_2}{4} - 1.194B_1 - 1.444B_2 + 9.3204 \in \left(a \frac{\partial f}{\partial r} \right) \right\}, \\
C_{44} &= 2.194T\beta K_T + \frac{e^2}{4\eta^4} \left\{ -1.194B_1 - 1.444B_2 + \frac{A_2}{4} \right\}, \quad (6)
\end{aligned}$$

where A_1 , B_1 , A_2 , and B_2 are short range force constants defined as

$$\begin{aligned}
\left(\frac{\partial^2 \phi'_1}{\partial r^2} \right)_{r=\eta} &= \frac{A_1 e^2}{8\eta^3}, & \left(\frac{1}{r} \frac{\partial \phi'_1}{\partial r} \right)_{r=\eta} &= \frac{B_1 e^2}{8\eta^3}, \\
\left(\frac{\partial^2 \phi'_2}{\partial r^2} \right)_{r=\eta\sqrt{2}} &= \frac{A_2 \sqrt{2} e^2}{8(\eta\sqrt{2})^3}, & \left(\frac{1}{r} \frac{\partial \phi'_2}{\partial r} \right)_{r=\eta\sqrt{2}} &= \frac{B_2 \sqrt{2} e^2}{8(\eta\sqrt{2})^3}. \quad (7)
\end{aligned}$$

The equilibrium condition $(d\phi(r))/dr = 0$ is written as

$$T\beta K_T = \frac{e^2}{4\eta^4} [1.165 \in (\in + 12f(r)) + B_1 + B_2], \quad (8)$$

where β is the coefficient of volume thermal expansion, a is the nearest neighbour distance, K_T is the bulk modulus, and $\eta = a[1 + \beta(T - T_0)]$.

3. Results and Discussion

In order to compute the values of elastic constants and bulk modulus with the help of the above described theory, one requires $f(r)$, $adf(r)/dr$, A_1 , B_1 , A_2 , and B_2 . Out of these the first four parameters are evaluated with the help of (6, 11) at $T = 300$ K using the input data from Table 1. The remaining two parameters A_2 and B_2 are evaluated by using (7). The computed parameters are used to evaluate the values SOE constants and bulk modulus for MgO, CaO, SrO, and BaO at different temperatures with the help of (6). The results are shown in the Tables 2, 3, 4, and 5.

It is interesting to note from Tables 2–5 that the values of C_{11} are decreasing with increase of temperature in all cases (MgO, CaO, SrO and BaO). The values of C_{11} for MgO and CaO are much better than previous theoretical results [5, 7] and very close to the experimental results [9]. Similarly the computed values of C_{12} of MgO, CaO, SrO, and BaO are decreasing slowly with the increase of temperature and are much better than the earlier computed values [5, 7] in case of MgO and CaO. The computed values of C_{44} are close to the experimental values [9] up to 1200 K and are better than the earlier reported values [5–7] in case of CaO. Our calculated values of C_{44} are not so good in case of MgO. This may be due to the reason that many body interactions do not show

TABLE 5: Calculated values of C_{11} , C_{12} , and C_{44} (in Gpa) for BaO at different temperatures T (in K).

T	C_{11}	C_{12}	C_{44}	K
300	121	50	38	73.6
400	117.97	49.57	38.03	72.37
500	114.98	49.16	38.06	71.1
600	112.03	48.76	38.12	69.85
700	109.11	48.37	38.17	68.62
800	106.22	48.01	38.24	67.41
900	103.36	47.65	38.32	66.22
1000	100.54	47.3	38.41	65.05
1100	97.74	46.96	38.5	63.89
1200	94.98	46.64	38.61	62.75
1300	92.24	46.33	38.72	61.63
1400	89.54	46.03	38.84	60.53
1500	86.86	45.74	38.97	59.44
1600	84.21	45.46	39.11	58.38
1700	81.58	45.19	39.26	57.32
1800	78.99	44.93	39.41	56.29
1900	76.42	44.69	39.57	55.26
2000	73.87	44.45	39.74	54.26

their contribution to the shear moduli C_{44} . Similar trend of variation of second-order elastic constants of AEO solids with pressure is obtained by Baltache et al. [9] and by Singh et al. [20]. Thus these AEOs show systematic variation in the values of SOE constant either with increase of pressure [9, 20] or with increase of temperature as compared to the values of these constants at ambient condition [10, 11].

On the other hand the values of bulk modulus are in excellent agreement with the experimental values [9] at different temperatures and are better than the earlier study which are based on the equation of state. The values of bulk modulus are decreasing at different temperatures as we move from lighter to heavier alkaline earth oxides. On the other hand, the value of bulk modulus is decreasing with the increase of temperature in all cases. The reason for this may be that the constant C_{11} is a longitudinal elastic constant (like Young's modulus) relating longitudinal stress and longitudinal strain. A longitudinal force causes the lattice to stretch. This causes a change in volume of the crystal lattice. It is well known that the internal energy is the function of volume (V) and temperature (T). The temperature dependence is both explicit via the Boltzmann factor and implicit via the static lattice energy and normal mode frequency. Both static lattice energy and normal mode frequency are the function of the volume (V), which heavily depend on temperature. Thus the constant C_{11} depends on the temperature. On the other hand, the constants C_{44} and C_{12} are shearing constant relating shearing stress to shearing strain. Shearing is caused by tangential force, and the lattice constant is unaffected by the shearing, and consequently the C_{44} and C_{12} depend less on temperature. This agreement demonstrates the validity of the contribution of many body interactions considered in developing the present theory.

The various results predicted in the present paper regarding the variation of the elastic constants with temperature for SrO and BaO up to 1800 K will be useful in analyzing the experimental data perhaps which are not yet available. Therefore the present study may be useful to study the elastic and thermal properties of alkaline earth chalcogenides and in geophysics.

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