

Pressure–Interatomic Separation–Temperature Relationship of Alkali Halides

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A new method for the determination of pressure–interatomic separation–temperature relationship is investigated and applied for some alkali halides. The method is developed by using the Mie–Grüneisen equation of state and the Anderson thermal pressure and an ionic model based on Harrison’s treatment of overlap repulsive potential which takes into account the interactions up to second neighbors. It is found that the new method yields satisfactory results in agreement with the available experimental data.

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1. Introduction

The understanding of the ionic solids at nonambient conditions is an integral part of physical sciences. Material scientists, solid state physicists, chemists, and solid earth geoscientists are routinely confronted with problems involving ionic solids at high pressure and high temperature [1]. In order to understand the behavior of ionic solids under the effect of high pressure and high temperature, considerable efforts have been made to determine the relationship between interatomic separation and temperature for alkali halides [2–7]. Moreover, at high pressure, relatively fewer efforts have been made.

The purpose of present paper is to develop a simple method for the determination of pressure–interatomic separation–temperature relationship. The calculations are performed within the framework of the Mie–Grüneisen equation of state and Anderson thermal pressure [1]. The potential model considers: (i) the long range electrostatic interactions in terms of Madelung’s energy; (ii) the short range overlap repulsive energy between nearest neighbors and next neighbors by adopting the analytical potential form derived by Harrison [8] based on quantum mechanical considerations; and (iii) the van der Waals dipole–dipole and dipole–quadrupole interactions. The method of analysis is described in Sect. 2. The results obtained are discussed and compared with the available experimental data for some alkali halides in Sect. 3.

2. Theory and method of calculation

The Mie–Grüneisen equation of state (EOS) can be expressed as follows [9]:

$$P = -\frac{d\phi}{dV} + P_{\text{th}}, \quad (1)$$

where ϕ is the lattice potential energy and V is the volume. In Eq. (1), the first term on right hand is the pressure due to volume dependence of electronic ground state energy (static pressure) and the second term is pressure due to vibration of nuclei (thermal pressure). P is the externally applied pressure. The correct expression for thermal pressure P_{th} can be taken from calculus as follows:

$$\left(\frac{\partial P}{\partial T}\right)_V = \left(\frac{\partial P_{\text{th}}}{\partial T}\right)_V = \alpha B_T, \quad (2)$$

where T is the temperature, α is the coefficient of volume thermal expansion and B_T is the isothermal bulk modulus. Upon integration we get

$$P_{\text{th}} = \int_0^T (\alpha B_T) dT. \quad (3)$$

This becomes $T\alpha B_T$ if the product αB_T is independent of T . This is approximately true above the Debye temperature θ_D [10]. However, Anderson [1] pointed out that the thermal pressure should be dependent on volume compression. It means that the product αB_T may not be a constant, so Eq. (3) should be modified as [1]:

$$P_{\text{th}} = \left[\alpha_0 B_{T_0} + \left(\frac{\partial B_T}{\partial T}\right)_V \ln \frac{V_0}{V} \right] T, \quad (4)$$

where α_0 and B_{T_0} are the values of α and B_T at reference temperature T_0 , V_0 — the volume at zero pressure and reference temperature T_0 . Substituting Eq. (4) into Eq. (1), we derived the following EOS:

$$P = -\frac{d\phi}{dV} + \left[\alpha_0 B_{T_0} + \left(\frac{\partial B_T}{\partial T}\right)_V \ln \frac{V_0}{V} \right] T. \quad (5)$$

Now using the relation $V = xr^3$, Eq. (5) can be rewritten as follows:

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$$P = -\frac{1}{3xr^2} \frac{d\phi}{dr} + \left[\alpha_0 B_{T_0} + \left(\frac{\partial B_T}{\partial T} \right)_V \ln \left(\frac{r_0}{r} \right)^3 \right] T, \quad (6)$$

where x is a constant which depends on the structure of solid. x equals 2 for NaCl-type and 1.54 for CsCl-type structures, and r is the interatomic separation.

For the calculation of ϕ , we use Harrison's potential form [8] for the overlap repulsive energy and also consider van der Waals (vdW) dipole-dipole and dipole-quadrupole interactions. Within the framework of Harrison's model the total lattice potential energy ϕ is expressed as follows:

$$\phi = -\frac{a_M Z^2 e^2}{r} - \frac{C}{r^6} - \frac{D}{r^8} + \phi_{\text{rep}}, \quad (7)$$

where the first term on the right-hand side of Eq. (7) is the electrostatic Coulomb energy with a_M as Madelung's constant which is equal to 1.7476 for NaCl-type structures and 1.7627 for CsCl-type structures, e — the charge of the electron, and Z — the valency. The second and third terms are van der Waals (vdW) dipole-dipole and dipole-quadrupole energies. The constants C and D are related to the dipole-dipole (c_{ij}) and dipole-quadrupole (d_{ij}) interaction coefficients as follows [11]:

$$C = S_{+-}c_{+-} + S_{++}c_{++} + S_{--}c_{--}, \quad (8)$$

$$D = T_{+-}d_{+-} + T_{++}d_{++} + T_{--}d_{--}, \quad (9)$$

where S_{ij} and T_{ij} are lattice sums which had been given by Tosi [12]. The subscripts $+$, $-$, $++$, $--$ represent the cation-anion, cation-cation, anion-anion interactions, respectively. The values of c_{ij} and d_{ij} are obtained from the Kirkwood-Muller formulae given below [11]:

$$c_{ij} = -\frac{6mc^2}{N} X_i X_j \left(\frac{X_i}{a_i} + \frac{X_j}{a_j} \right)^{-1}, \quad (10)$$

$$d_{ij} = -\frac{9mc^2}{Ne^2} c_{ij} \left(\frac{X_i}{n_i} + \frac{X_j}{n_j} \right), \quad (11)$$

where c is the velocity of light, a and X are the polarisabilities and molar susceptibilities, respectively. N is the Avogadro number. n_i and n_j are the number of outmost electrons. The values of C and D calculated from Eqs. (8)–(11) were used in the present work.

For the overlap repulsive energy, we use the analytical form proposed by Harrison [8]. The normalized charge density as used by Harrison from quantum mechanical consideration is

$$n(r) = \frac{6\mu^3}{\pi} \exp(-2\mu r), \quad (12)$$

where μ is related to the valence p and state energy (ε_p) as follows:

$$\varepsilon_p = -\frac{\hbar^2 \mu^2}{2m}, \quad (13)$$

where \hbar is Planck's constant h divided by 2π and m is the mass of an electron. The total overlap interaction has been considered as arising from three contributions,

viz., (i) the kinetic energy, (ii) the exchange energy and (iii) the Coulombian energy of electrons in the overlap region. These contributions to the overlap repulsive potential are given below [8]:

$$\phi^{\text{ke}} = 70.8\varepsilon_p \mu r \exp\left(-\frac{5\mu r}{3}\right), \quad (14)$$

$$\phi^{\text{ex}} = -2.728e^2 \mu^2 r \exp\left(-\frac{4\mu r}{3}\right), \quad (15)$$

$$\phi^{\text{coul}} = -6e^2 \mu^3 r^2 \exp(-2\mu r). \quad (16)$$

Harrison [8] assumed that the total overlap interaction is of the form of the kinetic energy term and can be expressed by an equation similar to that given by Eq. (14). So we can write the overlap repulsive potential as follows:

$$\begin{aligned} \phi_{\text{rep}} = & \frac{n_0 \hbar^2}{2m} \left[M \bar{\mu}^3 r \exp(-k\bar{\mu}r) \right. \\ & \left. + \frac{1}{2} M' \mu_1^3 r' \exp(-k\mu_1 r') + \frac{1}{2} M' \mu_2^3 r' \exp(-k\mu_2 r') \right]. \end{aligned} \quad (17)$$

For NaCl-type structures, $M = 6$ and $M' = 12$ are the numbers of first and second neighbor ions. Similarly, r and $r' = \sqrt{2}r$ are the first and second nearest neighbor distances. For CsCl-type structures $M = 8$, $M' = 6$, and $r' = (2/\sqrt{3})r$. The values of μ_1 and μ_2 are calculated using the valence p state energy (ε_p) given by Eq. (13), and $\bar{\mu}$ is the arithmetic average of μ_1 and μ_2 for the cation and anion.

In order to calculate lattice potential energy ϕ from Eq. (7), there remain only two unknown parameters, viz. n_0 and k which are obtained from the equilibrium condition and the following relations:

$$\left(\frac{d\phi}{dr} \right)_{r=r_0} = 0, \quad (18)$$

$$\left(\frac{d^2\phi}{dr^2} \right)_{r=r_0} = 9xr_0 B_{T_0}. \quad (19)$$

The potential parameters thus calculated are assumed to be independent of pressure. The input data required are given in Table I. Now, the values of $d\phi/dr$, the first derivative of the lattice energy can be calculated using Eq. (7) at any value of r , and finally the pressure P is calculated using Eq. (6) at different temperature. The values of pressure thus calculated for different values of r are given in Tables II–VI along with the available experimental data. At $P = 0$, Eq. (6) takes the following form:

$$T = \frac{1}{3xr^2} \frac{d\phi}{dr} / \left[\alpha_0 B_{T_0} + \left(\frac{\partial B_T}{\partial T} \right)_V \ln \left(\frac{r_0}{r} \right)^3 \right]. \quad (20)$$

Now the values of $d\phi/dr$ are calculated for increasing r and the corresponding temperature T is evaluated from Eq. (20) for some alkali halides. The results obtained are reported in Table VII along with the available experimental data.

Values of input parameters used in the present work [1, 11, and 13].

TABLE I

Crystal	r_0 [Å]	α_0 [10^{-4} K $^{-1}$]	B_{T_0} [kbar]	$(\partial B_T/\partial T)_V$	C [10^{-60} erg cm 6]	D [10^{-76} erg cm 8]	n_0	k	μ_1 [10 nm $^{-1}$]	μ_2 [10 nm $^{-1}$]
LiF	2.013	0.999	665	-0.051	46	26	3	1.34	3.962	2.112
LiCl	2.570	1.32	297	-0.027	317	221	11.6	1.41	3.962	1.799
LiBr	2.751	1.50	235	-0.025	594	286	9.5	1.34	3.962	1.716
LiI	3.006	1.80	172	-0.023	1265	584	61.6	1.57	3.962	1.619
NaF	2.317	0.96	465	-0.025	139	98	11.5	1.54	3.087	2.112
NaCl	2.820	1.19	240	-0.017	561	455	19.6	1.49	3.087	1.799
NaBr	2.989	1.26	199	-0.016	930	537	30.7	1.52	3.087	1.716
NaI	3.236	1.37	151	-0.013	1755	942	48.3	1.53	3.087	1.619
KCl	3.146	1.11	175	-0.012	607	285	70.9	1.67	2.487	1.799
KBr	3.289	1.16	148	-0.010	1854	962	112	1.71	2.487	1.716
KI	3.525	1.23	117	-0.008	2745	1430	64.5	1.57	2.487	1.619
RbCl	2.570	1.32	297	-0.011	317	221	11.6	1.41	3.962	1.799
RbBr	2.751	1.50	235	-0.009	594	286	9.5	1.34	3.962	1.716
RbI	3.006	1.80	172	-0.008	1265	584	61.6	1.57	3.962	1.619
CsCl	3.571	1.37	180	-0.015	333	357	974	2.08	2.116	1.799

TABLE II

Values of pressure (P in kbar) vs. interatomic separation for LiF crystal at different temperatures. The available experimental data [15] are given within parentheses.

298 K		573 K		873 K		1073 K	
r	P	r	P	r	P	r	P
2.013	0(0)	2.035	0(0)	2.066	0(0)	2.093	0(0)
2.003	9.98(10)	2.024	9.98(10)	2.053	9.99(10)	2.077	10.01(10)
1.994	19.94(20)	2.014	19.87(20)	2.041	19.91(20)	2.063	19.94(20)
1.985	29.72(30)	2.004	29.87(30)	2.030	29.96(30)	2.050	30.04(30)
1.977	39.84(40)	1.995	39.64(40)	2.019	39.84(40)	2.037	39.91(40)
1.969	49.88(50)	1.986	49.56(50)	2.009	49.72(50)	2.026	49.75(50)
1.961	59.59(60)	1.977	59.77(60)	1.999	59.47(60)	2.015	59.79(60)
1.954	69.75(70)	1.969	69.15(70)	1.944	69.23(70)	2.004	69.58(70)
1.946	79.46(80)	1.961	78.99(80)	1.982	79.45(80)	1.994	79.46(80)
1.940	89.16(90)	1.953	88.75(90)	1.973	88.97(90)	1.985	89.03(90)

3. Results and discussions

In order to judge the influence of the volume independence of thermal pressure of presented results, we have compared the values of pressure obtained by Eq. (3) and Eq. (4) with the experimental data [14] for NaCl crystal at 573 K (Table VIII). We note that the values of P calculated through Eq. (4) are in close agreement with experimental data. Thus, Eq. (4) proposed by the Anderson, seems to be more suitable for the thermal pressure than Eq. (3).

We have proposed a simple method to investigate the pressure–interatomic separation–temperature relationship in the wide range of temperatures and pressures. It is clear from Tables II–VII that the calculated values for all alkali halides are in good agreement with the experimental values [14–18], supporting the validity of the simple method.

For estimating the values of $d\phi/dr$ at r , we have used the potential energy expression given in the form of Eq. (7). Within the framework of this model, we have considered vdW dipole–dipole and dipole–quadrupole interactions. The dipole–dipole energy term, which arises

TABLE III

Values of pressure (P in kbar) vs. interatomic separation for NaF crystal at different temperatures. The available experimental data [15] are given within parentheses.

298 K		473 K		673 K		873 K		1073 K	
r	P	r	P	r	P	r	P	r	P
2.317	0(0)	2.331	0(0)	2.349	0(0)	2.369	0(0)	2.392	0(0)
2.301	9.99(10)	2.314	10.03(10)	2.331	9.98(10)	2.348	9.99(10)	2.370	10.00(10)
2.286	19.91(20)	2.299	19.89(20)	2.314	19.94(20)	2.330	19.95(20)	2.349	19.98(20)
2.273	29.88(30)	2.285	29.91(30)	2.299	29.95(30)	2.314	29.94(30)	2.331	29.94(30)
2.260	39.82(40)	2.272	39.71(40)	2.285	39.88(40)	2.299	39.92(40)	2.315	39.96(40)
2.249	49.65(50)	2.259	49.64(50)	2.272	49.81(50)	2.285	49.85(50)	2.300	49.87(50)
2.238	59.47(60)	2.248	59.51(60)	2.260	59.60(60)	2.273	59.71(60)	2.286	59.84(60)
2.228	69.21(70)	2.237	69.21(70)	2.249	69.37(70)	2.261	69.58(70)	2.273	69.55(70)
2.218	78.74(80)	2.226	78.96(80)	2.238	79.11(80)	2.250	79.30(80)	2.261	79.37(80)
2.210	88.80(90)	2.217	88.72(90)	2.228	88.99(90)	2.240	89.18(90)	2.249	89.44(90)

TABLE IV

Values of pressure (P in kbar) vs. interatomic separation for NaCl crystal at different temperatures. The available experimental data [14] are given within parentheses.

298 K		473 K		673 K		773 K	
r	P	r	P	r	P	r	P
2.820	0(0)	2.840	0(0)	2.868	0(0)	2.885	0(0)
2.801	5.0(5)	2.819	5.0(5)	2.844	5.0(5)	2.839	5.0(5)
2.784	10.0(10)	2.801	10.0(10)	2.821	10.0(10)	2.814	10.0(10)
2.769	14.9(15)	2.785	14.9(15)	2.804	14.9(15)	2.796	14.8(15)
2.754	19.8(20)	2.769	19.7(20)	2.788	19.8(20)	2.781	19.8(20)
2.740	24.6(25)	2.755	24.6(25)	2.771	24.5(25)	2.763	24.6(25)
2.728	29.8(30)	2.742	29.7(30)	2.755	29.7(30)	2.750	29.8(30)
2.717	34.6(35)	2.730	34.5(35)	2.745	34.7(35)		

TABLE V

Values of pressure (P in kbar) vs. interatomic separation for CsCl crystal at different temperatures. The available experimental data [15] are given within parentheses.

298 K		473 K		673 K		873 K	
r	P	r	P	r	P	r	P
3.571	0(0)	3.603	0(0)	3.646	0(0)	3.696	0(0)
3.514	9.96(10)	3.537	9.97(10)	3.568	9.99(10)	3.600	10.01(10)
3.468	19.91(20)	3.485	19.92(20)	3.509	19.25(20)	3.532	19.37(20)
3.430	29.33(30)	3.443	29.45(30)	3.462	29.47(30)	3.479	29.37(30)
3.397	38.98(40)	3.407	39.41(40)	3.422	39.29(40)	3.435	39.50(40)
3.368	48.72(50)	3.376	48.99(50)	3.388	49.25(50)	3.398	49.24(50)
3.343	58.97(60)	3.348	59.02(60)	3.358	58.97(60)	3.366	59.13(60)
3.319	68.58(70)	3.323	68.96(70)	3.332	69.01(70)	3.337	68.92(70)
3.298	78.66(80)	3.301	78.49(80)	3.307	78.58(80)	3.311	79.56(80)
3.279	88.29(90)	3.280	88.84(90)	3.284	88.97(90)	3.287	89.10(90)

TABLE VI

Values of pressure (P in kbar) vs. interatomic separation for some alkali halides at room temperature. The available experimental data [14, 16] are given within parentheses.

LiCl		LiBr		LiI	
r	P	r	P	r	P
2.570	0(0)	2.751	0(0)	3.006	0(0)
2.557	5.0(5)	2.733	5.0(5)	2.978	5.0(5)
2.545	10.1(10)	2.717	10.2(10)	2.954	10.0(10)
2.533	15.2(15)	2.700	15.2(15)	2.931	15.1(15)
2.522	20.5(20)	2.685	20.0(20)	2.911	20.0(20)
2.511	25.5(25)	2.672	24.9(25)	2.893	25.1(25)
2.501	30.5(30)	2.658	29.9(30)	2.876	30.6(30)
2.491	35.6(35)	2.646	34.7(35)	2.860	35.5(35)
2.481	41.0(40)	2.634	39.5(40)	2.847	40.5(40)
2.473	45.8(45)	2.624	44.3(45)	2.833	45.5(45)
NaBr		NaI			
r	P	r	P		
2.989	0(0)	3.237	0(0)		
2.966	5.0(5)	3.203	5.0(5)		
2.945	10.0(10)	3.173	9.9(10)		
2.925	14.8(15)	3.147	14.9(15)		
2.908	19.9(20)	3.124	19.9(20)		
2.892	24.6(25)	3.103	24.8(25)		
2.877	29.7(30)	3.084	29.8(30)		
2.863	34.6(35)	3.067	34.8(35)		
2.849	39.9(40)	3.049	39.9(40)		
2.837	44.6(45)	3.03	45.2(45)		

from the interaction between induced dipole moments of different atoms, is actually the first term in an infinite series of rapidly converging terms. The dipole–quadrupole term is interpreted as arising from the interaction of a dipole moment on one atom with a quadrupole on the other. Actually, there exists a third term, which varies inversely as the tenth power of interatomic distance, which is called the quadrupole–quadrupole term. In the present article we discuss only the dipole–dipole and dipole–quadrupole interactions because the quadrupole–quadrupole term is negligible in ionic crystals.

It should be mentioned that the overlap potential forms as given by Eq. (17) are based on Harrison’s quantum mechanical formulation and differ from the traditional Born–Mayer exponential forms [19, 20] in some important aspects. First, the pre-exponential factors appearing in Eq. (17) also depend directly on the interionic separation whereas in the Born–Mayer exponential forms, only the exponential factors depend on r . Secondly, ionic radii have been introduced arbitrarily as adjustable parameters in the Born–Mayer exponential forms. On the other hand, in Eq. (17) the pre-exponential as well as exponential factors depend on fundamental factors like Planck’s

TABLE VII

Values of temperature (T in K) vs. interatomic separation for some alkali halides at atmospheric pressure ($P = 0$). The available experimental data [17, 18] are given within parentheses.

KCl		KBr		KI	
r	T	r	T	r	T
3.116	0(0)	3.26	0(0)	3.489	0(0)
3.12	39(39)	3.28	173(175)	3.50	88(90)
3.14	220(222)	3.30	346(349)	3.52	225(230)
3.16	391(395)	3.32	507(512)	3.54	349(355)
3.18	490(492)	3.34	647(650)	3.56	466(475)
3.20	641(645)	3.36	777(780)	3.58	569(576)
3.22	775(778)	3.38	894(894)	3.60	669(680)
3.24	893(894)	3.40	1013(1015)	3.62	754(760)
3.26	1000(1002)			3.64	837(850)
3.27	1049(1052)			3.66	908(915)
RbCl		RbBr		RbI	
r	T	r	T	r	T
3.259	0(0)	3.41	0(0)	3.628	0(0)
3.26	36(40)	3.42	92(95)	3.64	101(105)
3.28	211(215)	3.44	231(235)	3.66	206(205)
3.30	316(320)	3.46	324(330)	3.68	326(315)
3.32	421(430)	3.48	418(425)	3.70	402(410)
3.34	539(550)	3.50	508(512)	3.72	470(475)
3.36	629(635)	3.52	693(699)	3.74	542(545)
3.38	754(770)	3.54	784(788)	3.76	613(615)
3.40	879(900)	3.56	872(880)	3.78	781(780)
3.42	1008(1020)	3.58	961(970)	3.80	850(845)

TABLE VIII

Values of pressure (P in kbar) obtained by Eq. (3) (column (a)) and Eq. (4) (column (b)) for NaCl crystal at 573 K. The experimental values (column (c)) are taken from Ref. [14].

r	P		
	(a)	(b)	(c)
2.831	0	0	0
2.811	5.0	5.0	5
2.794	10.0	10.0	10
2.780	14.7	14.9	15
2.764	19.7	19.8	20
2.750	24.6	24.7	25
2.738	29.4	29.8	30
percentage deviation at 30 kbar	2%	0.67%	

constant, electronic mass, and energy term values. Moreover, the exponential factors are different in different pair interactions, whereas in the Born–Mayer potential a common value of hardness parameters has been taken for the cation–anion, cation–cation, and anion–anion interactions. This is not justified for the reasons discussed by Shanker and Agrawal [11]. If one takes unequal values of hardness parameters for the crystal, then the number of parameters becomes too large to be determined from the input data for the lattice parameter and bulk modulus. Thus, the Harrison potential form is superior to the Born–Mayer exponential forms.

Finally, it should also be mentioned that the formulations proposed in the present study is of general nature and therefore its application may be extended to different classes of solids. The results of the present investigation also lead to the understanding of the equation of state based on the microscopic details of the theory of interionic potentials.

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