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# Analysis of Isothermal Bulk Modulus for DI Atomic Solids at High Pressure

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**ABSTRACT:** Chopelas-Boehler approximation for the volume dependence of the Anderson-Grüneisen parameter yields an analytical formula for the volume dependence of thermal expansivity ( $\alpha$ ) whereas the Anderson-Isaak equation gives an expression which can not be integrated analytically. a new form of the isothermal equations of state is used which is integrated analytically. The values of interatomic distances ( $r$ ) volume ( $V/V_0$ ), isothermal bulk modulus ( $B_T$ ) and the thermal expansivity ( $\alpha$ ) are calculated with the change of pressure for alkali halides at temperature of 300(K) and compare with available experimental data.

**KEYWORDS :** Thermoelastic properties, interatomic distances, Alkali bromide, bulk modulus, Thermal expansivity, High pressure behaviour.

## I. INTRODUCTION

The isothermal equation of state (EOS) gives us a useful information about the relationship between the changes in pressures and volume at fixed temperature. The-theoretical studies of EOS at high temperature and pressures are very important in the field of science and engineering works and also gives information on the non-linear thermal expansion and compressions of solids[1,2]. Isothermal equation of state is very valuable in basic and applied science [3]. Thermodynamic and thermoelastice properties is very essential properties of solids because it is a fundamental interest to geophysical and geochemical theory of the interior of the earths. Many expressions gives the thermodynamic properties such as the pressure dependence [4,- 8] and temperature dependence [9-19] of the interatomic distances , volume expansion and Bulk Modulus ( $B_T$ ), Thermal expansivity ( $\alpha$ ) of solids in a large range of temperature and pressure.

In this paper, we have discussed a new analytical isothermal EOS based on the approximation for the volume dependence of the Anderson Grüneisen parameter  $\delta_T$  along isotherm [4]. Calculate the values of interatomic distances( $r$ ) , volume expansion ( $V/V_0$ ) ,isothermal bulk modulus ( $B_T$ ),thermal expansivity ( $\alpha$ ) with change of pressure at room temperature of each solids.

The method of analysis is given in sect-2 and the systematic study and discussion of results are given in sect-3.

## II. METHOD OF ANALYSIS

On the basis of an analysis of experimental data, Chopelas and Boehler investigate relationship [4,22] for the isothermal variation of  $\delta_T$  with volume.

$$\delta_T + 1 = \left( \delta_T^0 + 1 \right) \frac{V}{V_0} \quad (1)$$

Eq.(1) chosen by Anderson et al because of the convenience of the power law in the mathematical expressions inherent in thermodynamic identities [4].

$$\frac{\alpha}{\alpha_0} = \left( \frac{V}{V_0} \right)^{\delta_T} \quad (2)$$

and

$$\frac{\alpha}{\alpha_0} = \frac{B_T^0}{B_T} \quad (3)$$

We use these identities and some relations to find out the equations of states in the previous work [21], and we directly used these equations given as-

1.To calculate thermal expansivity-

$$\frac{\alpha}{\alpha_0} = \frac{V_0}{V} \exp \left[ \left( \delta_T^0 + 1 \right) \left( \frac{V}{V_0} - 1 \right) \right] \quad (4)$$

2.Isothermal bulk modulus-

$$\frac{B_T}{B_T^0} = \frac{V}{V_0} \exp \left[ \left( \delta_T^0 + 1 \right) \left( 1 - \frac{V}{V_0} \right) \right] \quad (5)$$

3.Volume expansion-

$$\frac{V}{V_0} = 1 - \frac{1}{\left( \delta_T^0 + 1 \right)} \ln \left[ 1 + \left( \delta_T^0 + 1 \right) \frac{P - \Delta P_{th}}{B_T^0} \right] \quad (6)$$

Where  $\Delta P_{th} = \alpha_0 B_0 (T - T_0)$

4.Interatomic distances-

$$\left( \frac{r}{r_0} \right)^3 = 1 - \frac{1}{\left( \delta_T^0 + 1 \right)} \ln \left[ 1 + \left( \delta_T^0 + 1 \right) \frac{P - \alpha_0 B_T^0 (T - T_0)}{B_T^0} \right] \quad (7)$$

where r is interatomic distances and  $r_0=r$  at  $P = 0$ .

### III. RESULTS AND DISCUSSION

In the present study we consider thermodynamic and thermoelastice properties of LiBr, NaBr, KBr, RbBr, and CsBr . For these solids the data are used at temperature of 300 (K) and pressure approximate limit of 0 to 25.0 (GPa). Isothermal bulk modulus  $B_T$  for all the solids under study decreases almost linearly with the increasing temperatures and the values of  $B_T$  increases linearly with the increasing pressure[21]. On the other hand the thermal expansivity  $\alpha$  goes on increasing in the high temperature region approaching the melting temperature but in the increasing to the high pressure region the thermal expansivity linearly decreases.

Table 1 : Input data used in calculations compiled from references [8,16,17,21,22]

Diatomic solids	$r_0(10^{-1}nm)$	$B_T^0$ (GPa )	$\alpha_0 (10^{-4}k^{-1})$	$\delta_T^0$
LiBr	2.751	23.5	1.50	7.01
NaBr	2.989	19.9	1.26	6.23
KBr	3.300	14.8	1.16	5.94
RbBr	3.445	23.5	1.08	6.71
CsBr	2.720	15.9	1.39	5.71

Table 2 : comparison of Experimental values and Calculated values of  $V/V_0$ with the change of pressure for alkali bromides from Eq.(6)[21] .

Press P (GPa)	LiBr		NaBr		KBr		RbBr		CsBr	
	$V/V_0$		$V/V_0$		$V/V_0$		$V/V_0$		$V/V_0$	
	Cal	Exp [20]	Cal	Exp [20]	Cal	Exp [20]	Cal	Exp [20]	Cal	Exp [20]
0.0	1.0000	----	1.0000	----	1.0000	----	1.0000	---	1.0000	----
0.5	0.9804	0.9811	0.9769	0.9768	0.9696	0.9712	0.9803	0.8267	0.9715	0.9695
1.0	0.9634	0.9632	0.9571	0.9561	0.9446	0.9450	0.9632	0.8067	0.9475	0.9432



1.5	0.9485	0.9463	0.9398	0.9374	0.9233	0.9215	0.9481	0.7883	0.9269	0.9207
2.0	0.9351	0.9306	0.9245	0.9206	0.9047	0.8023	0.9346	0.7714	0.9088	0.9012
2.5	0.9231	0.9159	0.9106	0.9053	0.8882	0.7867	0.9223	0.7561	0.8927	0.8844
3.0	0.9121	0.9023	0.8980	0.8913	0.8734	0.7727	0.9111	0.7424	0.8781	0.8696
3.5	0.9020	0.8897	0.8865	0.8784	0.8601	0.7602	0.9008	0.7303	0.8648	0.8563
4.0	0.8926	0.8782	0.8759	0.8663	0.8478	0.7493	0.8913	0.7198	0.8526	0.8440
4.5	0.8839	0.8677	0.8660	0.8547	0.8365	0.7399	0.8824	0.7108	0.8414	0.8319
5.0	0.8758	-----	0.8568	-----	0.8260	-----	0.8741	-----	0.8309	-----
10.0	0.8148	-----	0.7879	-----	0.7495	-----	0.8114	-----	0.7537	-----
15.0	0.7740	-----	0.7422	-----	0.6998	-----	0.7693	-----	0.7031	-----
2.0	0.7433	-----	0.7079	-----			0.7376	-----	0.6654	-----
25.0	0.7187	-----					0.7121	-----		

Table 3 :comparison of Experimental values and Calculated values of  $r(10^{-1}nm)$  with the change of pressure for alkali bromides from Eq.(7) [21].

Press P (GPa)	LiBr		NaBr		KBr		RbBr		CsBr	
	$r(10^{-1}nm)$		$r(10^{-1}nm)$		$r(10^{-1}nm)$		$r(10^{-1}nm)$		$r(10^{-1}nm)$	
	Cal	Exp [20]	Cal	Exp [20]	Cal	Exp [20]	Cal	Exp [20]	Cal	Exp [20]
0.0	2.7510	-----	2.9890	-----	3.3000	-----	3.4450	-----	2.7200	-----
0.5	2.7329	2.7336	2.9658	2.9657	3.2662	3.2680	3.4222	3.2332	2.6939	2.6921
1.0	2.7170	2.7168	2.9456	2.9446	3.2379	3.2384	3.4022	3.2070	2.6715	2.6675
1.5	2.7029	2.7008	2.9278	2.9253	3.2134	3.2113	3.3843	3.1824	2.6520	2.6461
2.0	2.6902	2.6858	2.9118	2.9077	3.1917	3.0664	3.3682	3.1595	2.6347	2.6273
2.5	2.6786	2.6716	2.8971	2.8915	3.1721	3.0464	3.3534	3.1385	2.6190	2.6109
3.0	2.6679	2.6583	2.8837	2.8765	3.1544	3.0282	3.3397	3.1194	2.6047	2.5962
3.5	2.6580	2.6459	2.8713	2.8626	3.1383	3.0118	3.3271	3.1023	2.5914	2.5829
4.0	2.6488	2.6344	2.8599	2.8494	3.1233	2.9973	3.3154	3.0874	2.5792	2.5705
4.5	2.6401	2.6239	2.8490	2.8366	3.1093	2.9847	3.3043	3.0745	2.5679	2.5581
5.0	2.6320	-----	2.8389	-----	3.0963	-----	3.2939	-----	2.5571	-----
10.0	2.5695	-----	2.7607	-----	2.9976	-----	3.2132	-----	2.4753	-----
15.0	2.5258	-----	2.7062	-----	2.9298	-----	3.1566	-----	2.4187	-----
20.0	2.4920	-----	2.6639	-----			3.1126	-----	2.3746	-----
25.0	2.4642	-----					3.0764	-----		



Table 4: Variation of Calculated values of isothermal bulk modulus ( $B_T$ ) and thermal expansivity  $\alpha_0$  ( $10^{-4}k^{-1}$ ) with pressure P (GPa) for alkali bromides at temperature of 300(K) from Eq.(5,4)[21].

Press P (GPa)	Temperature 300 (K)									
	LiBr		NaBr		KBr		RbBr		CsBr	
	( $B_T$ )	( $\alpha$ )	( $B_T$ )	( $\alpha$ )	( $B_T$ )	( $\alpha$ )	( $B_T$ )	( $\alpha$ )	( $B_T$ )	( $\alpha$ )
0.0	23.5000	1.5000	19.9000	1.2600	14.8000	1.1600	23.5000	1.0800	15.9000	1.3900
0.5	26.9558	1.3076	22.9739	1.0914	17.7206	0.9688	26.8157	0.9464	18.7021	1.1817
1.0	30.3525	1.1613	25.9725	0.9654	20.5345	0.8360	30.0611	0.8442	21.4272	1.0314
1.5	33.6711	1.0468	28.9011	0.8675	23.2690	0.7378	33.2433	0.7634	24.0686	0.9182
2.0	36.9567	0.9538	31.7560	0.7895	25.9418	0.6617	36.3646	0.6979	26.6460	0.8294
2.5	40.1632	0.8776	34.5853	0.7249	28.5586	0.6011	39.4558	0.6432	29.1599	0.7579
3.0	43.3399	0.8133	37.3597	0.6711	31.1205	0.5516	42.4920	0.5972	31.6352	0.6986
3.5	46.4715	0.7585	40.3405	0.6256	33.6101	0.5107	45.4839	0.5579	34.0644	0.6487
4.0	49.5834	0.7109	42.7538	0.5864	36.0816	0.4758	48.4243	0.5241	36.4487	0.6063
4.5	52.6438	0.6695	45.4071	0.5522	38.5050	0.4458	51.3459	0.4942	38.7773	0.5699
5.0	55.6579	0.6333	48.0145	0.5222	40.8957	0.4197	54.2242	0.4681	41.0887	0.5378
10.0	84.4061	0.4176	72.6620	0.3450	63.1017	0.2720	81.6231	0.3109	62.5665	0.6101
15.0	111.1718	0.3171	95.2473	0.2632	83.1839	0.2063	107.0636	0.2371	81.9625	0.4618
20.0	136.5255	0.2581	116.4137	0.2153	-----	-----	131.0725	0.1936	99.8948	0.2212
25.0	160.7583	0.2192	-----	-----	-----	-----	154.0338	0.1647	-----	-----

The relations [ Eq.(4) and Eq.(5)] proposed [21] in the present study yield more satisfactory results for thermal expansivity  $\alpha$  this is in the increasing high pressure region linearly decreases and isothermal bulk modulus  $B_T$  linearly increasing in the high pressure region ,i.e. pressure increases ,isothermal bulk modulus  $B_T$  increases and the thermal expansivity  $\alpha$  decreases. Data used at the temperature of 300(K) and the pressure range 0 to 25.0 (GPa) for LiBr and RbBr, pressure range 0 to 20.0 (GPa) for NaBr and CsBr, pressure range 0 to 15.0 (GPa) for KBr. Under pressure dependent study for solids in table no.4. the extrapolated values of  $\alpha$  and  $B_T$  at temperature of 300 (K) and pressure range approx 0 to 25.0 (GPa) are expected to be more reliable. It is found that in high pressure region  $\alpha$  decreases and  $B_T$  increases for all alkali bromides. Considerably at high pressure the values of volume expansion  $V_{(P)}/V_{(300)}$  and interatomic distances have been calculated using the equations (6,7) in the present study for these solids up to the pressure approx 25.0 (GPa) at the temperature of 300(K) , i.e. pressure increases linearly ,interatomic distances ( r) and volume ( $V/V_0$ ) both are linearly decreases, the results are listed in the table no. (2,3) are given that a good agreement with the available experimental results based on the density measurements [20].



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