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Thermal pressure and thermal expansivity of solids at high temperatures

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ABSTRACT

Thermal pressure and thermal expansivity for sodium chloride and potassium chloride solids has been calculated at high temperatures using various Equation of State. The results from these calculations have been compared with the experimental data and the results are found to present close agreement with the experimental data. A close agreement between present study and the experiment data reveals the validity of the present work. The values of thermal pressure and thermal expansivity at high temperatures are useful to understand the thermo-elastic behavior of solids.

Keywords: Equation of State, Thermal expansivity, Thermal pressure

INTRODUCTION

Thermal pressure is a physical quantity of central importance[1] for investigating thermo-elastic properties of materials at high temperatures [2-3]. The volume expansion of solids is directly related to thermal pressure P_{th} due to rise in temperature[4-5]. The study of elastic properties is essential for examining and understanding of the dynamics of earth's deep interior, structure and composition of earth's lower mantle and in seismic studies.[1]

The elasticity offers more information that the volume in interpreting the temperature dependence of equation of state (EOS) because the compressibility is defined by the derivative of volume6. The study of high pressure and high temperature behavior of solids demonstrate that the thermal expansivity (α) is a very important quantity needed for geophysical data analysis and condensed matter physics 7-9, so various theoretical attempts have been made to solve this problem.

In order to understand the thermodynamic and thermo-elastic behavior of solids at high temperatures, it is necessary to have reliable values of elastic constants corresponding to such temperatures. The common methodology to determine the temperature dependence of elastic constants is to use the volume expansion data for solids at high temperatures. In the present study, we calculated the thermal pressure and thermal expansivity for sodium chloride and potassium chloride.

THEORY

To calculate thermal pressure P_{th} , we are using these equations

$$\Delta P_{th} = K_0\left(\frac{V}{V_0} - 1\right) - \frac{1}{2}K_0(K_0' + 1)\left(\frac{V}{V_0} - 1\right)^2 \quad (1)$$

$$\Delta P_{th} = \frac{K_0\left(\frac{V}{V_0} - 1\right) - \frac{1}{2}K_0(K_0' - 1)\left(\frac{V}{V_0} - 1\right)^2}{\frac{V}{V_0}} \quad (2)$$

$$\Delta P_{th} = \frac{K_0\left(\frac{V}{V_0} - 1\right) - \frac{1}{2}K_0(K_0' - 3)\left(\frac{V}{V_0} - 1\right)^2}{\left(\frac{V}{V_0}\right)^2} \quad (3)$$

Where K_0 and K_0' are isothermal bulk modulus and its pressure derivatives both at P = 0 Equation (1) is derived by Shanker et al[10] , equation (2) has been obtained by Singh[11] , equation (3) has been obtained by Shanker and Kushwah [12] . Anderson gave one more relation for P_{th} using Anderson Grüneisen parameter

$$\Delta P_{th} = \frac{K_0}{M}\left[1 - exp.\left\{-\delta_T^0\left(\frac{V}{V_0} - 1\right)\right\}\right] \quad (4)$$

Here the parameter M represents the slope of the plot between isothermal bulk modulus versus change in thermal pressure. Where δ_T^0 is the value of Anderson Grüneisen parameter δ_T at initial temperature. Thermal pressure evaluated through equation (4) based on the Anderson Grüneisen parameter is a volume dependent term [13, 14] can be considered more accurate and may be used to understand high temperature behavior of solids.

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One more equation, we are using for calculating thermal pressure using Kushwah logrithmic EOS[15-16].

$$\Delta P_{th} = B_0 - B_1 exp\left(-\frac{V/V_0}{B_2}\right) \quad (5)$$

Where B_0, B_1 and B_2 constant and their values are:

		B_0	B_1	B2
For	NaCl	3.702	2471.01	0.1537
	KCl	2.591	1866.23	0.1519

For thermal expansivity, we are using these equations [10, 17-19]

$$\frac{\Delta}{V_0} = \frac{V}{V_0} - 1 = \frac{1-\left[1-2\left(\frac{K_0'+1}{K_0}\right)P_{th}\right]^{\frac{1}{2}}}{(K_0'+1)} \quad (6)$$

The factor $(K_0' + 1)$ in numerator if we replace it with $(K_0' - 1)$ we get a new equation – Suzuki equation i.e

$$\frac{V}{V_0} - 1 = \frac{1-\left[1-2\left(\frac{K_0'-1}{K_0}\right)P_{th}\right]^{\frac{1}{2}}}{(K_0'-1)} \quad (7)$$

Recently Kumar [20] has shown that Suzuki relation [21] as well as Tait [18] and Murnaghan EOS [19] can be used to obtain relation for thermal expansivity.

Tait EOS is expressed as:

$$\frac{V(0,T)}{V(0,T_R)} = [1 - A\,\alpha(0,T_R)(T - T_R)]^{-\frac{1}{A}} \quad (8)$$

Murnaghan approach

$$\frac{V(0,T)}{V(0,T_R)} = [1 - (A-1)\,\alpha(0,T_R)(T - T_R)]^{-\frac{1}{A-1}} \quad (9)$$

RESULT AND DISCUSSION

Values of input parameters used in present calculation are given in table 1: [1,22,23]

Solids	P_{th}				
	K_0	K_0'	K_∞'	M	δ_T^0
NaCl	24	5.38	3.23	5.96	5.78
KCl	17	5.46	3.28	5.91	5.71

Table 1. For Thermal expansivity (T_R - 300K)

	NaCl			KCl		
T(K)	α $10^{-5}/K$	A(K_0) GPa	P_{th}	A $10^{-5}/K$	A(K_0) GPa	P_{th}
300	11.8	24.0	0.00	11.0	17.0	0.00
350	12.2	23.2	0.14	11.3	16.4	0.09
400	12.7	22.4	1.28	11.7	15.9	0.19
450	13.2	21.6	0.43	12.1	15.4	0.28
500	13.7	20.8	0.57	12.6	14.7	0.37
550	14.3	19.9	0.71	13.2	14.2	0.47
600	14.8	19.0	0.85	13.7	13.7	0.56
650	15.4	18.1	0.99	14.2	13.2	0.65
700	16.0	17.3	1.13	14.7	12.6	0.75
750	16.6	16.5	1.27	15.2	12.0	0.84
800				15.7	11.5	0.93
850				16.2	10.9	1.02

Table 2. Thermal Pressure for NaCl computed from (a) equation (1), (b) equation (2), (c) equation (3), (d) equation (4), (e) equation (5 and (f) experimental data [1]

		ΔP_{th}					
T(K)	V/V_0	(a)	(b)	(c)	(d)	(e)	(f)
300	1.0000	0.00	0.00	0.00	0.00	0.00	0.00
350	1.0060	0.14	0.14	0.14	0.14	0.15	0.14
400	1.0123	0.28	0.28	0.28	0.28	0.29	0.28
450	1.0188	0.42	0.42	0.42	0.41	0.44	0.43
500	1.0256	0.56	0.55	0.57	0.55	0.58	0.57
550	1.0328	0.70	0.68	0.71	0.70	0.72	0.71
600	1.0402	0.84	0.81	0.85	0.83	0.86	0.85
650	1.0480	0.98	0.93	0.99	0.98	1.00	0.99
700	1.0561	1.11	1.04	1.13	1.12	1.13	1.13
750	1.0645	1.23	1.15	1.23	1.25	1.28	1.27
800	1.0732	1.35	1.25	1.39	1.39	1.41	
850	1.0832	1.46	1.35	1.52	1.52	1.54	
900	1.0916	1.56	1.43	1.64	1.66	1.67	
950	1.1012	1.64	1.49	1.76	1.78	1.79	
1000	1.1112	1.72	1.55	1.88	1.90	1.91	
1050	1.1214	1.79	1.59	1.98	2.03	2.03	
1100	1.1319	1.83	1.62	2.08	2.14	2.13	
1150	1.1427	1.87	1.63	2.18	2.26	2.24	
1200	1.1538	1.88	1.62	2.27	2.27	2.35	

Thermal Pressure for KCl computed from (a) equation (1), (b) equation (2), (c) equation (3), (d) equation (4), (e) equation (5) and (f) experimental data [1]

		ΔP_{th}					
T(K)	V/V_0	(a)	(b)	(c)	(d)	(e)	(f)
300	1.0000	0.00	0.00	0.00	0.00	0.00	0.00
350	1.0054	0.09	0.09	0.09	0.09	0.09	0.09
400	1.0112	0.18	0.18	0.18	0.18	0.19	0.19
450	1.0172	0.28	0.27	0.28	0.27	0.28	0.28
500	1.0235	0.37	0.36	0.37	0.36	0.37	0.37
550	1.0301	0.46	0.45	0.46	0.45	0.47	0.47
600	1.0370	0.55	0.53	0.55	0.55	0.56	0.56
650	1.0442	0.64	0.62	0.65	0.64	0.66	0.65
700	1.0517	0.73	0.70	0.74	0.73	0.75	0.75
750	1.0594	0.82	0.77	0.83	0.83	0.84	0.84
800	1.0675	0.90	0.84	0.92	0.92	0.93	0.93
850	1.0759	0.97	0.90	1.01	1.01	1.02	1.02
900	1.0847	1.05	0.96	1.10	1.10	1.11	
950	1.0938	1.11	1.02	1.18	1.19	1.19	
1000	1.1032	1.17	1.06	1.26	1.28	1.28	
1050	1.1129	1.21	1.10	1.33	1.37	1.36	
1100	1.1230	1.26	1.12	1.41	1.45	1.44	
1150	1.1334	1.29	1.14	1.48	1.53	1.51	
1200	1.1437	1.31	1.14	1.54	1.61	1.59	

Table 3. Thermal expansivity V/V_0 for sodium chloride and potassium chloride (a) calculated from equation (6), (b) calculated from equation (7) due to Suzuki, (c) calculated

from equation (8) Tait Approach, (d) calculated from equation (9) Murnaghan Approach and (e) based on experimental data[1].

NaCl					
T(K)	(a)	(b)	(c)	(d)	(e)
300	1.0000	1.0000	1.0000	1.0000	1.0000
350	1.0059	1.0059	1.0066	1.0066	1.0060
400	1.0121	1.0120	1.0151	1.0149	1.0123
450	1.0191	1.0187	1.0262	1.0258	1.0188
500	1.0259	1.0251	1.0414	1.0403	1.0256
550	1.0331	1.0318	1.0644	1.0614	1.0328
600	1.0407	1.0387	1.1026	1.0933	1.0402
650	1.0489	1.0459	1.2277	1.1606	1.0480
700	1.0577	1.0533			1.0561
750	1.0674	1.0611			1.0645

KCl					
T(K)	(a)	(b)	(c)	(d)	(e)
300	1.0000	1.0000	1.0000	1.0000	1.0000
350	1.0054	1.0054	1.0060	1.0060	1.0054
400	1.0116	1.0115	1.0130	1.0129	1.0112
450	1.0175	1.0171	1.0215	1.0213	1.0172
500	1.0236	1.0230	1.0320	1.0314	1.0235
550	1.0307	1.0296	1.0455	1.0442	1.0301
600	1.0375	1.0358	1.0623	1.0598	1.0370
650	1.0447	1.0422	1.0842	1.0794	1.0442
700	1.0533	1.0496	1.1131	1.1039	1.0517
750	1.0617	1.0565	1.1540	1.1353	1.0594
800	1.0710	1.0638	1.2246	1.1801	1.0675
850	1.0814	1.0714	1.3846	1.2410	1.0759

The above calculations for thermal pressure and thermal expansivity for NaCl and KCl have been shown by the various graphs as follows:

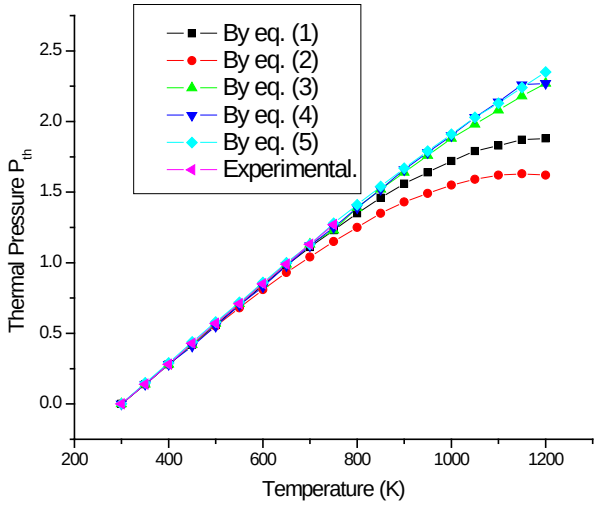

Figure1. Thermal Pressure (P_{th}) versus Temperature (K)for NaCl.

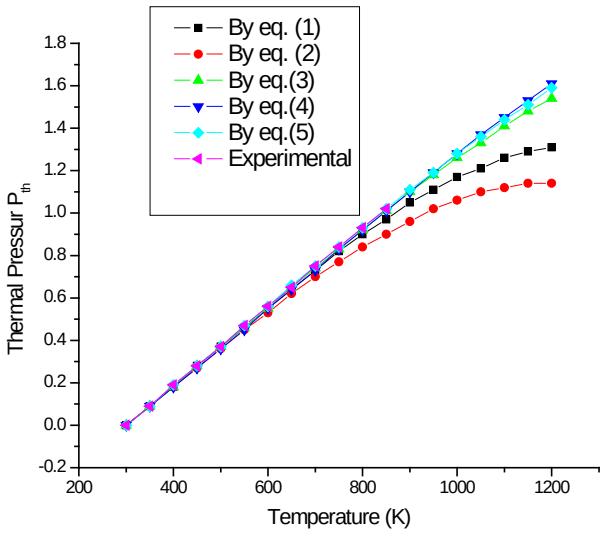

Figure 2. Thermal Pressure (P_{th}) versus Temperature (K) for KCl.

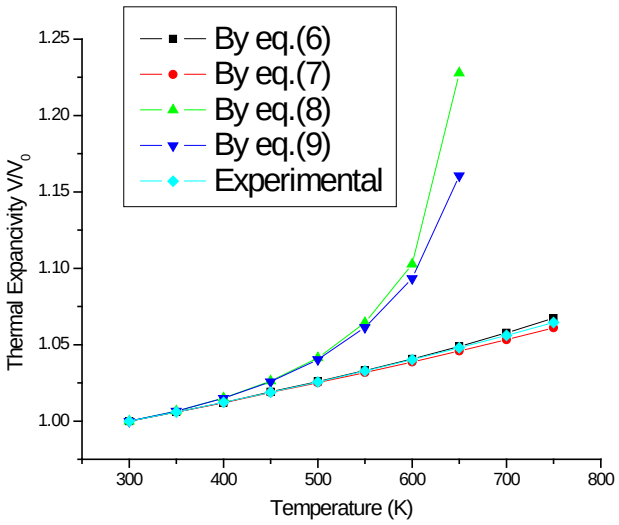

Figure 3.Thermal Expansivity (V/V_0) versus Temperature (K) for NaCl.

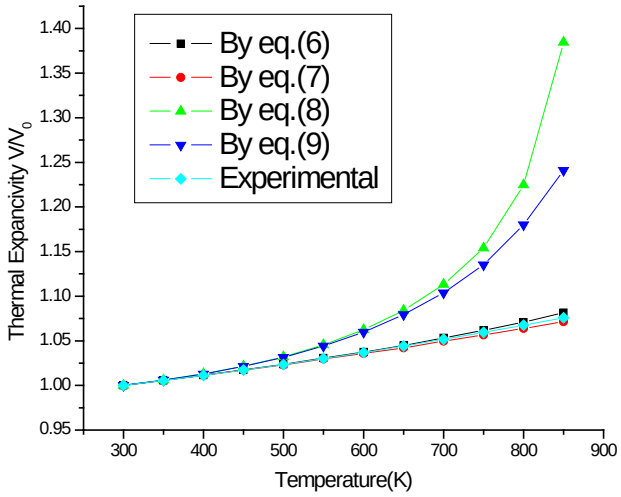

Figure 4. Thermal Expansivity (V/V_0) versus Temperature (K) for KCl.

CONCLUSION

In conclusion, the results calculated for thermal pressure and thermal expansivity agree with experimental data for Sodium chloride and Potassium Chloride but in case of thermal pressure, the results calculated by eq. 2 deviates above the temperature 550 K and in case of thermal expansivity, the results calculated by Tait and Murnaghan Approach does not agree well with experimental data.

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REFERENCES AND NOTES

1. O.L. Anderson . Equation of state of Solids for Geophysics and ceramic sciences, Oxford University Press, New York, **1995**.
2. S.S. Kushwah, P. Kumar, J. Shanker . Analysis of pressure-volume-temperature relationship for some alkali halide crystals. *Physica B* **1996,** 229, 85.
3. L.M. Thomas , J. Shanker . Temperature dependence of elastic constants and thermal expansion coefficient for NaCl crystals. *Phys. Stat. Sol. B* **1996,** 195, 361.
4. S.S. Kushwah, J. Shanker. A comparative study of equation of state for MgO. *Physica B* **1998,** 253, 90.
5. J. Shanker, S.S. Kushwah. High pressure isothermal equation of state for material with pressure derivative of the isothermal bulk modulus less than four. *High temperature-High pressure* **2001,** 33, 207.
6. S.P. Singh, J. Singh. *J. Pure and App. Sci. & Tech.* **2012,** 2(2), 54-63.
7. O.L. Anderson. Accurate thermal expansivity measurements in the range 1500-2000K are needed for minerals, *Int. J. Thermophys.* **1991,** 12, 757.
8. O.L. Anderson, D. Isaak, H. Oda. High-temperature elastic constant data on minerals relevant to geophysics, *Rev. Geophys.* **1992,** 30, 57.
9. S. Yamamoto, I. Ohno, O.L. Anderson. High temperature elasticity of sodium Chloride, *J. Phys. Chem. Solids*. **1987,** 48, 143.
10. J. Shanker, S.S. Kushwah, P. Kumar. Theory of thermal expansivity and bulk modulus for MgO and other minerals at high temperatures. *Physica B* **1997,** 233, 78.
11. K.S. Singh. Relationships between thermal pressure and volume expansion for solids at high temperature, *High temperature- High pressure* **2002**, 34(4), 379.
12. J. Shanker, S.S. Kushwah. High-pressure isothermal equation of state for materials with pressure derivative of isothermal bulk modulus less than four, *High temperature- High pressure* **2001,** 33(2), 207.
13. S.K. Srivastava. Temperature dependence of volume expansion ratio for ionic solids. *Physica B* **2005,** 363, 122.
14. B.P. Singh. *Phys. Chem. Miner* **2005,** 32/7, 482.
15. S.S. Kushwah, H.C. Shrivastava, K.S. Singh. Studu of pressure-volume relationships and higher derivatives of bulk modulus based on generalized equation of state. *Physica B* **2007**, 388, 20.
16. S.S. Kushwah , Y.S. Tomar. Relationships between volume thermal expansion and thermal pressurebased on the Stacey reciprocal K-primed EOS. *Int. J. Pure and App. Phys.* **2011**, 49, 99-103.
17. R.E. Gibson, O.H. Loffer. *J. Am. Chem. Soc.* **1941**,63, 898.
18. P.J.Tait. *Phys . Chem.* **1991,** 2, 1.
19. F.D. Murnaghan. Finite deformation of an elastic solid (John Wiley and Sons, Inc., New York) **1951,** chap -4.
20. M.Kumar. A comparative study of Suzuki and Kumar formulation for thermal expansivity. *Indian J. Pure & Appl. Phys.* **2004,** 42, 67.
21. I.Suzuki, S.Okajima, K.Seya. *J. Phys. Earth* **1979,** 27, 63.
22. B.P. Singh, H. Chandra. Temperature dependence of elastic moduli and isobaric volume expansion of ionic solids. *Physica B* **2005,** 358,1.
23. R.S. Singh, D. Sahrawat. Analysis of high pressure properties of metals using equations of state. *J. Integr. Sci. Technol*., **2014**, 2(2), 42-48