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Thermal expansivity of geophysical minerals at high temperatures

Monika Panwar, S.K. Sharma, Sanjay Panwar

Abstract— A new model for investigating the value of thermal expansivity is presented. It has been found that the values obtained in the present study are consistent with the experimental data. The excellent agreement between results obtained and experimental data show the validity of the present work.

Index Terms—Thermal pressure, Thermal expansivity, Bulk modulus, Equation of state, Volume expansion ratio, Geophysical minerals.

1 Introduction

Thermal expansivity is a very important parametric quantity for interpreting the thermal and elastic properties of minerals at high temperatures because it has been emphasized [1] that most of the serious errors in the calculations of thermodynamic function arise due to uncertainty of thermal expansivity at high temperatures. Many researchers [2-5] have been made to estimate the temperature dependence of thermal expansivity to keep in mind its linear as well as non-linear dependence. Thermal expansivity is necessary parameter for solving many problems of material science and geophysics and many thermal and elastic properties can also be derived from it. Thermal expansivity may also be defined as

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

where V, T and P are the volume, temperature and pressure respectively. Method of analysis is seen in section 2, result and discussion in section 3 and conclusion are presented in section 4.

2 METHOD OF ANALYSIS

Anderson [6] used the following relationship to estimate the value of thermal pressure

$$P_{th} = \alpha K_T (T - T_0) \tag{2}$$

$$\alpha = \frac{P_{th}}{K_T (T - T_0)} \tag{3}$$

where P_{th}, α, and K_T are thermal pressure, thermal expansivity and isothermal bulk modulus and T_0 is room temperature or reference temperature. Thermal pressure is a physical quantity of central importance for investigating the thermo elastic properties of materials at high temperatures [6-8]. The volume expansion of solids due to the rise in temperature is directly related to thermal pressure [9, 10]. The equation of state (EoS) is effectively important in studying the properties of solids under high pressure and high temperature. The EoS yields pressure–volume–temperature (P–V–T) relationship for solids and helps in estimating a variety of properties under different conditions of pressure and temperature

$$P(V,T) = P(V,T_0) + \Delta P \tag{4}$$

where V is the volume, T the temperature and T_0 is initial value of temperature taken here equal to 300 K. In writing Eq. (2) and (3), it has been assumed that the thermal pressure is a function of temperature only [1]. At atmospheric pressure i.e. at P (V, T) = 0, we have

$$P(\mathrm{V},\mathrm{T}) = -\Delta P_{th} \tag{5}$$

It should be mention that Stacey reciprocal K-primed (SRKP) equation of state (EoS) [11-13] is valid for both isothermal bulk modulus as well as adiabatic bulk modulus. The Stacey reciprocal K-primed (SRKP) equation of state (EoS) [11] can be written as follows

$$\frac{1}{K'} = \frac{1}{K_0'} + \left(1 - \frac{K_\infty'}{K_0'}\right)\frac{P}{K} \tag{6}$$

Eq. (6) on integration gives an expression for bulk modulus which has further been integrated to obtained [11]

- Monika Panwar, Department of Physics, MMEC, Maharishi Markandeshwar University, Ambala, Haryana-133207, India. PH+918059110033. E-mail: monikaverma05@gmail.com
- S.K. Sharma,, Department of Physics, Shivalik Institute of Engineering and Technology, Aliyaspur, Ambala, Haryana-133206, India. PH+918295055704. E-mail: sav31@rediffmail.com
- Sanjay Panwar, Department of Physics, MMEC, Maharishi Markandeshwar University, Ambala, Haryana-133207, India. PH+918607715111. E-mail: dr.spanwar@gmail.com

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$$\ln\frac{V}{V_0} = \frac{K_0'}{K_\infty'^2}\ln\left(1 - K_\infty'\frac{P}{K}\right) + \left(\frac{K_0'}{K_\infty'} - 1\right)\frac{P}{K} \tag{7}$$

Now, replacing P by $-\Delta P_{th}$, Eq. (5) can be written as:

$$\ln\frac{V}{V_0} = \frac{K_0'}{K_\infty'^2}\ln\left(1 + K_\infty'\frac{\Delta P_{th}}{K}\right) - \left(\frac{K_0'}{K_\infty'} - 1\right)\frac{\Delta P_{th}}{K} \tag{8}$$

where K_T is the isothermal bulk modulus, K_0' is the first pressure derivative of isothermal bulk modulus at atmospheric pressure i.e. $P = 0$ and K_∞' is an important parameter which is first pressure derivate of isothermal bulk modulus at infinite pressure i.e. $P \to \infty$. Which can be determine by using [13-17]

$$K_\infty' = 0.6K_0'$$

where K_0' is the first pressure derivative of isothermal bulk modulus at atmospheric pressure i.e. $P = 0$ and at room temperature.

Pallavi Sinha et al. [18] used the following data to calculate P_{th} data

$$P = K_0\left[\left(\frac{1+m+m^2/2}{K_\infty'}\right)\left\{\left(\left(\frac{V}{V_0}\right)^{-K_\infty'} - 1\right) + \frac{m(m+1)}{K_0'-K_\infty'}\left(\left(\frac{V}{V_0}\right)^{K_0-K_\infty} - 1\right\} - \frac{m^2}{2(2K_0-K_\infty)}\left(\left(\frac{V}{V_0}\right)^{2K_0-K_\infty} - 1\right)\right]\right] \tag{9}$$

where

$$m = \frac{K_0' - K_\infty'}{K_0'}$$

and other parameter are having their usual meaning and the following relationship have been used to be investigate the value of isothermal bulk modulus K_T by Pallavi Sinha et al. [18]

$$\left(\frac{K_T}{K_0}\right) = \left(\frac{V}{V_0}\right)^{-K_\infty'} exp\left[\left(\frac{K_0'-K_\infty'}{K_0'}\right)\left\{1 - \left(\frac{V}{V_0}\right)^{K_0'}\right\}\right] \tag{10}$$

3 RESULTS AND DISCUSSIONS

We have computed the values of volume expansion by using the Eq. (8) values of input parameter used in the calculation are shown in Table -2, for geophysical minerals MgO, Al_2O_3 and Mg_2SiO_4. The values of ΔP_{th} have been taken from Anderson [6] to calculate volume expansion through Eq. (8) is shown in Table-1 and the results obtained through it. A close agreement has been found for all geophysical minerals used in the present study. The values of isothermal bulk modulus (K_T) have been predicted from Eq. (10). Results obtained shown the consistency with the experimental data as shown in Table -2, 3, and 4 for MgO, Al_2O_3 and Mg_2SiO_4.

As it is clear from Eq. (3) to investigate the values of thermal expansivity, the values of thermal pressure, K_T and T_0 are necessary. By using the concept $P = -\Delta P_{th}$ Eq. (9) takes the form

$$P_{th} = K_0\left[\frac{m^2}{2(2K_0-K_\infty)}\left\{\left(\frac{V}{V_0}\right)^{2K_0-K_\infty} - 1\right\} - \left(\frac{1+m+m^2/2}{K_\infty'}\right)\left\{\left(\left(\frac{V}{V_0}\right)^{-K_\infty'} - 1\right) - \frac{m(m+1)}{K_0'-K_\infty'}\left\{\left(\frac{V}{V_0}\right)^{K_0-K_\infty} - 1\right\}\right]\right] \tag{11}$$

where all the parameters are having their as usual meaning. The predicted values through Eq. (11) are compared with experimental data Anderson [6] in Table-2, 3 and 4 for MgO, Al_2O_3, Mg_2SiO_4. Comparison between results obtained and experimental data show the good agreement for all geophysical minerals. Using the Eq. (10) and (11), Eq. (3) becomes

$$\alpha = \frac{\left[\frac{m^2}{2(2K_0-K_\infty)}\left\{\left(\frac{V}{V_0}\right)^{2K_0-K_\infty} - 1\right\} - \left(\frac{1+m+m^2/2}{K'_\infty}\right)\left\{\left(\left(\frac{V}{V_0}\right)^{-K'_\infty} - 1\right) - \frac{m(m+1)}{K'_0-K'_\infty}\left\{\left(\frac{V}{V_0}\right)^{K_0-K_\infty} - 1\right\}\right]\right]}{\left(\frac{V}{V_0}\right)^{-K_\infty'} exp\left[\left(\frac{K_0'-K_\infty'}{K_0'}\right)\left\{1 - \left(\frac{V}{V_0}\right)^{K_0'}\right\}\right](T - T_0)} \tag{12}$$

The results obtained through Eq. (12) are shown in Table-2, 3 and 4 with the experimental data for MgO, Al_2O_3, and Mg2SiO4 respectively. Consistency the results obtained from Eq. (12) and experimental data validate the present approach. For direct vision ΔP_{th} vs T are plotted in Figures-1, 2 and 3 for MgO, Al_2O_3, Mg_2SiO_4 respectively. It is clear from these figures that the results obtained through Eq. (11) are competent with experimental data [6]. α vs T are plotted in Figures- 4, 5 and 6 for MgO, Al_2O_3, and Mg_2SiO_4 respectively. An excellent agreement between results obtained through Eq. (12) and experiment data shows the validity of present model.

4 CONCLUSIONS

In the present study we introduce a new model to predict the values of thermal expansivity for geophysical minerals such as MgO, Al_2O_3, and Mg2SiO4. It is conclude that the results obtained in the present study support the validity of the present model.

Table 1 – Values of input data used in calculations: isothermal bulk modulus K_0 (GPa) and pressure derivative of isothermal bulk modulus K_0' are at T = 300 K and atmospheric pressure.

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Parameters	K_0 (GPa)	K'_0 (GPa)	K'_∞ (GPa)	m
MgO	162	4.15	2.49	0.400
Al_2O_3	252	3.99	2.39	0.401
Mg_2SiO_4	127	5.40	3.24	0.400

Table 2 — Values of volume thermal expansion, thermal pressure (P_{th}), and thermal expansivity (α) for MgO as a function of temperature

T (K)	$\frac{V}{V_0}$ Eq. (8)	$\frac{V}{V_0}$ Exp. Ref.[6]	P_{th} (GPa) Eq. (11)	P_{th} (GPa) Exp. Ref.[6]	α (10^{-5} K^{-1}) Eq. (12)	α (10^{-5} K^{-1}) Exp. Ref. [6]
300	1.0000	1.0000	0.00	0.00	0.00	0.00
400	1.0034	1.0033	0.54	0.54	3.39	3.40
500	1.0071	1.0073	1.13	1.12	3.59	3.59
600	1.0111	1.0112	1.75	1.73	3.77	3.77
700	1.0153	1.0153	2.38	2.35	3.91	3.92
800	1.0196	1.0196	3.02	2.98	4.05	4.05
900	1.0241	1.0240	3.67	3.61	4.17	4.18
1000	1.0287	1.0284	4.32	4.24	4.29	4.30
1100	1.0334	1.0332	4.96	4.87	4.41	4.41
1200	1.0382	1.0380	5.61	5.50	4.52	4.53
1300	1.0431	1.0428	6.26	6.12	4.63	4.64
1400	1.0482	1.0476	6.90	6.74	4.74	4.75
1500	1.0533	1.0528	7.54	7.36	4.86	4.87
1600	1.0586	1.0581	8.18	7.97	4.98	4.98
1700	1.0644	1.0635	8.87	8.58	5.14	5.15
1800	1.0696	1.0688	9.45	9.20	5.23	5.24

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Table 3 — Values of volume thermal expansion, thermal pressure (P_{th}), and thermal expansivity (α) for Al_2O_3 as a function of temperature

T (K)	$\frac{V}{V_0}$ Eq. (8)	$\frac{V}{V_0}$ Exp. Ref.[6]	P_{th} (GPa) Eq. (11)	P_{th} (GPa) Exp. Ref.[6]	α (10^{-5} K^{-1}) Eq. (12)	α (10^{-5} K^{-1}) Exp. Ref. [6]
300	1.0000	1.0000	0.00	0.00	0.00	0.00
400	1.0018	1.0018	0.45	0.45	1.80	1.80
500	1.0039	1.0040	0.98	0.98	1.98	1.98
600	1.0063	1.0063	1.56	1.55	2.12	2.12
700	1.0088	1.0088	2.17	2.15	2.23	2.23
800	1.0114	1.0114	2.79	2.76	2.32	2.32
900	1.0143	1.0142	3.47	3.43	2.43	2.43
1000	1.0169	1.0168	4.09	4.01	2.48	2.48
1100	1.0197	1.0195	4.74	4.64	2.54	2.54
1200	1.0227	1.0223	5.41	5.27	2.61	2.61
1300	1.0257	1.0252	6.07	5.90	2.67	2.67
1400	1.0288	1.0279	6.75	6.53	2.74	2.74
1500	1.0318	1.0308	7.42	7.16	2.79	2.79
1600	1.0349	1.0337	8.08	7.79	2.84	2.84
1700	1.0381	1.0364	8.74	8.42	2.89	2.89
1800	1.0412	1.0394	9.38	9.01	2.93	2.93

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Table 4 — Values of volume thermal expansion, thermal pressure (P_{th}), and thermal expansivity (α) for Mg_2SiO_4 as a function of temperature

T (K)	$\frac{V}{V_0}$ Eq. (8)	$\frac{V}{V_0}$ Exp. Ref.[6]	P_{th} (GPa) Eq. (11)	P_{th} (GPa) Exp. Ref.[6]	α (10^{-5} K^{-1}) Eq. (12)	α (10^{-5} K^{-1}) Exp. Ref. [6]
300	1.0000	1.0000	0.0000	0.00	0.00	0.00
400	1.0029	1.0028	0.3602	0.36	2.88	2.88
500	1.0060	1.0059	0.7496	0.75	3.05	3.05
600	1.0094	1.0094	1.1571	1.16	3.20	3.20
700	1.0128	1.0129	1.5628	1.57	3.30	3.30
800	1.0164	1.0164	1.9819	1.98	3.41	3.41
900	1.0201	1.0199	2.3955	2.40	3.51	3.51
1000	1.0239	1.0238	2.8149	2.83	3.61	3.61
1100	1.0275	1.0277	3.1970	3.22	3.66	3.66
1200	1.0320	1.0320	3.6716	3.69	3.83	3.83
1300	1.0361	1.0363	4.0912	4.13	3.93	3.93
1400	1.0406	1.0407	4.5330	4.56	4.06	4.06
1500	1.0449	1.0451	4.9461	5.00	4.16	4.17
1600	1.0492	1.0498	5.3466	5.43	4.26	4.26
1700	1.0541	1.0547	5.7929	5.87	4.41	4.41

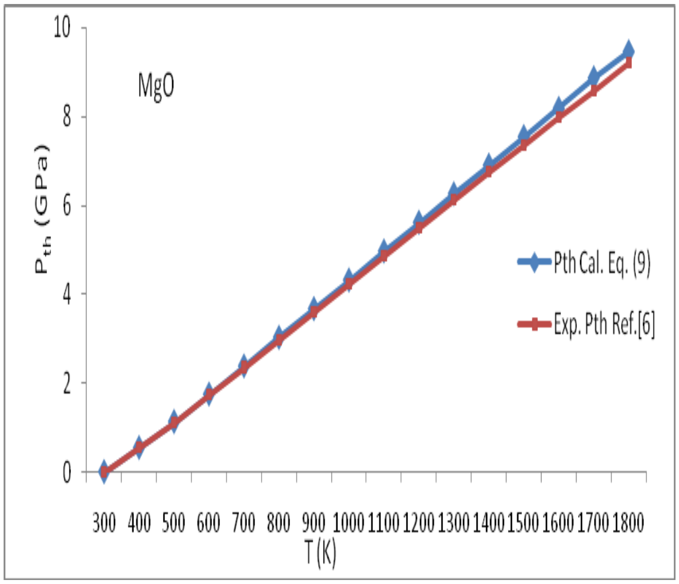

Figure 1: Comparison of theoretical and experimental value of temperature dependence of volume expansion ratio calculated by various Eqs. for MgO

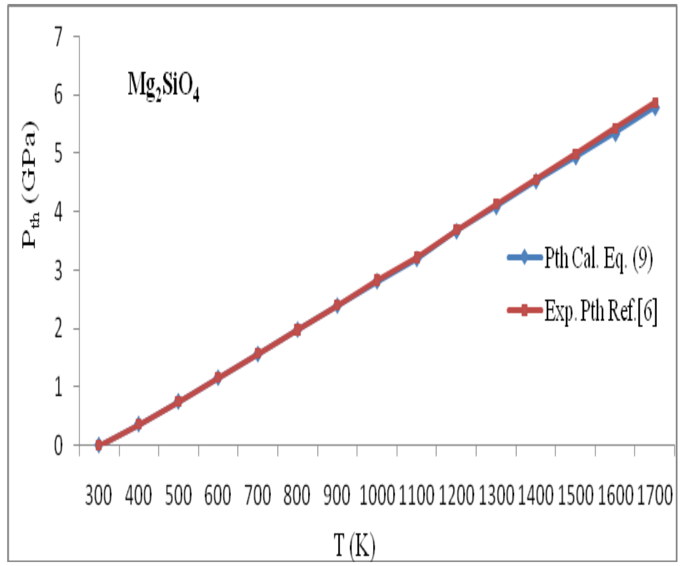

Figure 3: Comparison of theoretical and experimental value of temperature dependence of volume expansion ratio calculated by various Eqs. for Mg_2SiO_4

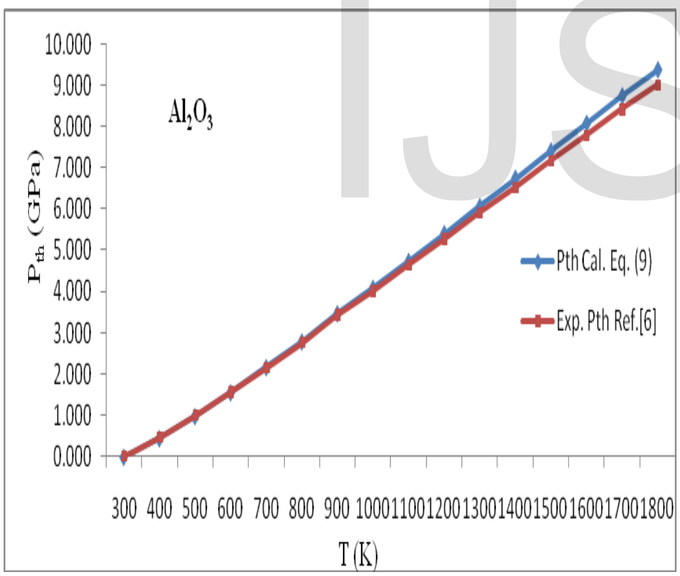

Figure 2: Comparison of theoretical and experimental value of temperature dependence of volume expansion ratio calculated by various Eqs. for Al_2O_3

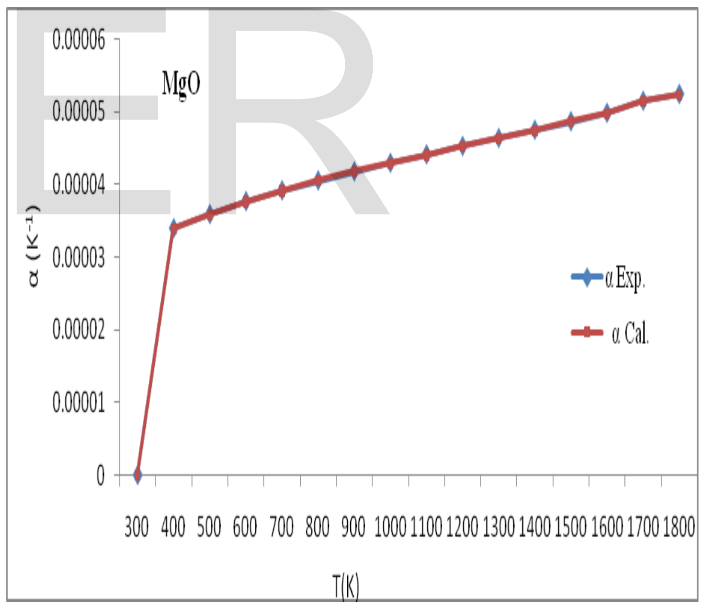

Figure 4: The graph between thermal expansivity (α) and temperature for MgO between calculated values and experimental data

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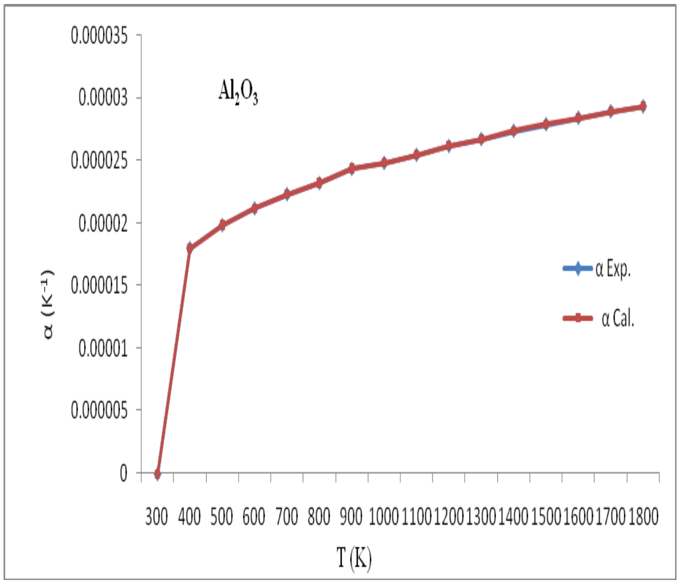

Figure 5: Thermal expansivity (α) for Al_2O_3 calculated in present study and experimental data

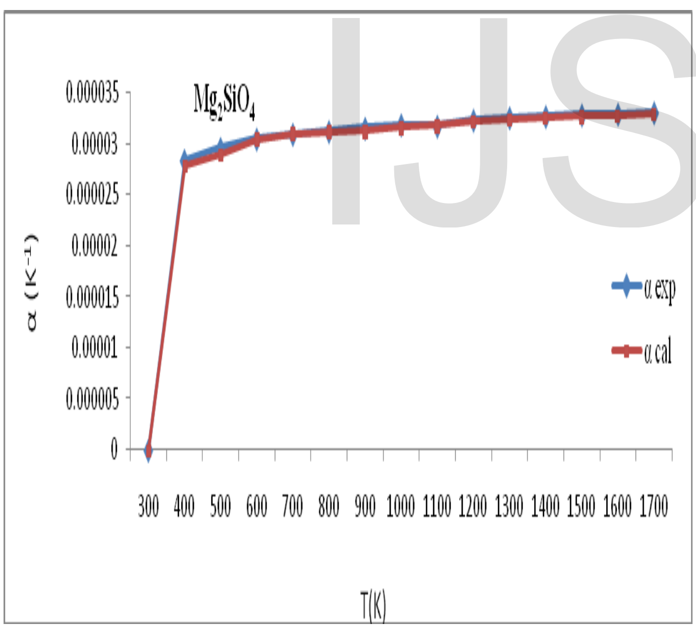

Figure 6: Thermal expansivity (α) for Mg_2SiO_4 calculated in present study and experimental data

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