ANALYSIS OF THERMO-ELASTIC PROPERTIES OF Mg_2SiO_4

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ABSTRACT

In the present study, we have developed the new expression for temperature dependence of elastic properties using thermodynamic relations. The proposed equation of state is applied to investigate the study elastic constants of Mg_2SiO_2. The computed values of second order elastic constants have shown a good agreement with available experimental results. It is concluded that a new expression for SOE constants is capable to predict the elastic properties of minerals under high temperature conditions.

***Keywords*:** EOS, SOEC, Mg_2SiO_2, High temperature.

INTRODUCTION

The variation of elastic properties of solids under high pressure and high temperature are of great interest to researchers in many fields such as geophysics, materials sciences. The study of elastic properties of minerals 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[1-3]. The behaviors of elastic properties under the effect of high pressure and high temperature have attracted the attention of experimental[1-4] as well as theoretical workers [5-10].

In the present study, a new relation for temperature dependence of elastic constants are developed using equation of state for the temperature dependence of bulk modulus and the formulation derived fromTallon's method based on thermodynamic analysis. The proposed equation of state is applied to investigate the elastic constants of Mg_2SiO_2. The computed values of second order elastic constants have shown a good agreement with available experimental results and far better than the earlier theoretical study.

2. Theory

The thermodynamical expression for thermal expansivity α is given by Anderson[1]

$$\alpha_T = \alpha_0 [1 - \alpha_0 \delta_T (T - T_0)]^{-1} \quad \dots (1)$$

Where α_0 is the value of α at $T = T_0$, the room temperature and δ_T is the value of Anderson-Grüneisen parameter related to temperature dependence of K_T, isothermal bulk modulus as follows.

$$\delta_T = -\frac{1}{\alpha K_T}\left(\frac{\partial K_T}{\partial T}\right)_P \quad \dots (2)$$

Assuming that δ_T is independent of temperature and taking coefficient of volume thermal expansion defined as follows:

$$\alpha = -\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \quad \dots (3)$$

The linear relationship for the variation of bulk modulus (K_T) with temperature has been reported by Kushwah et.al[11].

$$K_T = K_0\left[1 - \alpha_0 \delta_T^0 (T - T_0)\right] \quad \dots (4)$$

On integrating Eq. (1), we have

$$\int_{V_0}^{V} \frac{dV}{V} = \int_{T_0}^{T} \frac{\alpha_0}{[1 - \alpha_0 \delta_T (T - T_0)]} dT$$

Then, we have

$$V = V_0 [1 - \alpha_0 \delta_T (T - T_0)]^{-1/\delta_T} \quad \dots (5)$$

One of the most widely used thermodynamic approximations is that product αK_T remains constant[12], i.e.

$$\alpha K_T = \text{Constant.} \quad \dots (6)$$

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Where α and K_T are the coefficient of volume thermal expansion and isothermal bulk modulus, respectively

On differentiating Eq. (6) with respect to T, at constant pressure, we have:

$$\alpha\left(\frac{dK_T}{dT}\right)_P + K_T\left(\frac{d\alpha}{dT}\right)_P = 0 \quad \ldots(7)$$

Or

$$\left(\frac{dK_T}{dT}\right)_P = -\frac{K_T}{\alpha}\left(\frac{d\alpha}{dT}\right)_P \quad \ldots(8)$$

The isothermal Anderson-Grüneisen parameter δ_T is defined as follows[3]

$$\delta_T = -\frac{1}{\alpha K_T}\left(\frac{\partial K_T}{\partial T}\right)_P \quad ..(9)$$

Substituting the value of Eq. (8) in Eq. (9), we get:

$$\delta_T = \frac{1}{\alpha^2}\left(\frac{\partial \alpha}{\partial T}\right)_P \quad \ldots(10)$$

Where α is the coefficient of volume thermal expansion and defined as follows:

$$\alpha = -\frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \quad \ldots(11)$$

From of Eq. (10) and Eq. (11), we get:

$$\ldots(12) \quad \delta_T = \frac{V}{\alpha}\left(\frac{\partial \alpha}{\partial V}\right)_P$$

The empirical temperature dependence of δ_T is considered as follows[13]

$$\delta_T = \delta_T^0 (X)^k \quad \ldots(13)$$

Where δ_T^0 is the value of Anderson-Grüneisen parameter at $T = T_0$, and $X = T/T_0$, T_0 is the reference temperature. *k*is the new dimensionless parameter which can be calculated from the slope of the graph plotted between $\log \delta_T^0$ and $\log(T/T_0)$. If we thus substitute the value of δ_T from Eq. (13) in Eq. (10), we can be obtained the modified expression for thermal expansion coefficient as follows:

$$\delta_T^0 X^k = \frac{1}{\alpha^2}\left(\frac{\partial \alpha}{\partial T}\right)_P \quad \ldots(14)$$

Or $$\delta_T^0\left(\frac{T}{T_0}\right)^k = \frac{1}{\alpha^2}\left(\frac{\partial \alpha}{\partial T}\right)_P \quad \ldots(15)$$

By integrating Eq. (15), we have

$$\frac{\delta_T^0}{T_0^k}\frac{T_0^{k+1}}{(k+1)} = -\frac{1}{\alpha_T} + C \quad \ldots(16)$$

Where C is an integration constant evaluated from initial conditions at $T = T_0$ and $\alpha_T = \alpha_0$,

$$\frac{\delta_T^0}{T_0^k (k+1)}(T^{k+1} - T_0^{k+1}) = \frac{1}{\alpha_0} - \frac{1}{\alpha_T} \quad \ldots(17)$$

The final expression for thermal expansivity is thus obtained as

$$\frac{\alpha_T}{\alpha_0} = \left[1 - \frac{\alpha_0 \delta_T^0}{T_0^k (k+1)}(T^{k+1} - T_0^{k+1})\right]^{-1} \quad \ldots(18)$$

If the empirical temperature dependence of δ_T is assumed then Eq.(9) at P = 0, may also written as follows:

$$-\left(\frac{\partial K_T}{\partial T}\right)_P = \alpha_0 K_0 \delta_T \quad \ldots(19)$$

Using Eq.(13), we have

$$\delta_T^0\left(\frac{T}{T_0}\right)^k = -\frac{1}{\alpha_0 K_0}\left(\frac{\partial K_T}{\partial T}\right)_P \quad \ldots(20)$$

Integrating Eq. (20), we have

$$\int_{K_0}^{K_T} dK_T = -\alpha_0 K_0 \delta_T^0 \int_{T_0}^{T}\left(\frac{T}{T_0}\right)^k dT \quad \ldots(21)$$

Thus, we get the final expression for the bulk modulus K_T is

$$K_T = K_0\left[1-\frac{\alpha_0\delta_T^0}{T_0^k(k+1)}(T^{k+1}-T_0^{k+1})\right] \quad ...(22)$$

Where K_0 is the value of K_T at initial temperature $T = T_0 = 300K$ and at atmospheric pressure.

Grover et al[14].used a non-standard definition[15] of δ_T known as isothermal Anderson-Grüneisen parameter and recalled it the parameter *g* as given as below:

$$g = -\frac{V_0}{K_T}\left(\frac{\partial K_T}{\partial V}\right)_P \quad ... (23)$$

Where V_0 is the value of V at $P = 0$. Equation (23) when generalized read as follows:

$$g_M = -\frac{V_0}{M}\left(\frac{\partial M}{\partial V}\right)_P \quad ... (24)$$

Where M represent any of the elastic moduli[15] has expressed equation (24) as follows:

Following the method of generalization as used by Tallon[15] to get the relevant expression for elastic constants may be written collectively as follows:

$$C_{ij} = C_{ij0}\left(1-\frac{\alpha_0\delta_{ij0}}{T_0^k(k+1)}\{T^{k+1}-T_0^{k+1}\}\right) \quad ...(25)$$

Where δ_{ij0} is given by equation (9) and evaluated using the method discussed in detail by Singh et al., Kumar and Bedi[16-20].

RESULT AND DISCUSSIONS

The values of input parameters used in calculations of thermophysical and thermoelastic properties for Mg_2SiO_4 using the data reported by Anderson and Isaak[2] and listed in the Table-1.

	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{23}	C_{31}	C_{12}
C^0_{ij}	330.0	200.0	236.0	67.2	81.5	81.2	72.1	68.0	66.2
	δ_{11}	δ_{22}	δ_{33}	δ_{44}	δ_{55}	δ_{66}	δ_{23}	δ_{31}	δ_{12}
δ_{ij}	4.56	5.07	5.50	7.11	6.60	6.95	3.20	5.10	6.00

	K_0	α_0	δ_T^0
	127.30	2.72	5.94

Table-1: Values of input parameters[1, 3]. C^0_{ij}(GPa), K_0 (GPa), δ_{ij}(dimensionless),α_0 ($10^{-5}K^{-1}$) and δ_T^0 (dimensionless).

The temperature dependence of thermal expansivity and thermal expansion are calculated by eq. (1), eq. (18) and eq. (5) from room temperature to 1800K. The results are shown in Figure 1-2. The values of isothermal bulk modulus (K_T) calculated from eq. (4) has been reported by Kushwah et.al[11].and eq. (22) at different temperature and atmospheric pressure for Mg_2SiO_4. The results are shown in Fig. 3 along with the experimental data[2].In eq. (22) needs only three input parameters such as Anderson-Grüneisen parameter (δ_T^0), volume thermal expansion coefficient (α_0) at zero pressure and the thermo-elastic parameter *k* which can be calculated from the graph between $\log(\delta_T^0)$ vs. $\log(T/T_0)$ and shown in Figure 4. The value of dimensionless thermoelastic parameter *k* = -0.087 for Mg_2SiO_4 has been used in present calculation. It has been noted that the values of bulk modulus (K_T) calculated from eq. (4) and eq. (22) deviate significantly from experimental data[2] but eq. (22) has been shown better agreement with the experimental data as compared with eq. (4). A good agreement obtained for the temperature dependence of bulk modulus, encouraged the authors to extend these theory for the study of the temperature dependence of second order elastic constants. Now, Eq. (22) may be generalized in the following manner, by using the method of generalization[15]. Equation (22) may be written for the second-order elastic constants (SOEC) in the form of Eq. (25) which is used to compute the temperature dependence of SOEC i.e. C_{ij}. Thus the results obtained using eq. (25) are plotted in Figs 5-7 for the second order elastic constants i.e. C_{ij} and compared with experimental data[2] for Mg_2SiO_4 under study present reasonably good agreement with the available experimental data[3].The percentage deviations calculated at highest temperature at T =1800K are reported in Table 2 and also shown by bar diagram in Fig.8.

C_{ij}	C_{11}	C_{22}	C_{33}	C_{44}	C_{55}	C_{66}	C_{23}	C_{31}	C_{12}	K_T
Max % Dev.	0.14	-2.29	2.27	0.08	1.9	-0.12	0.77	1.57	1.56	-1.73

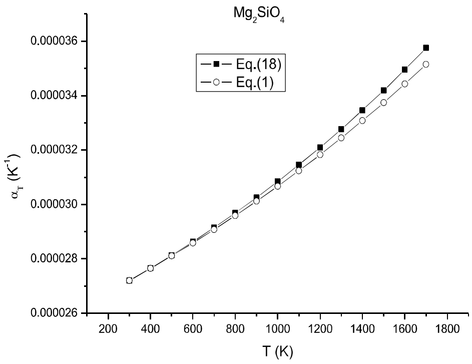

Fig.1-Temperature dependence of α_T.

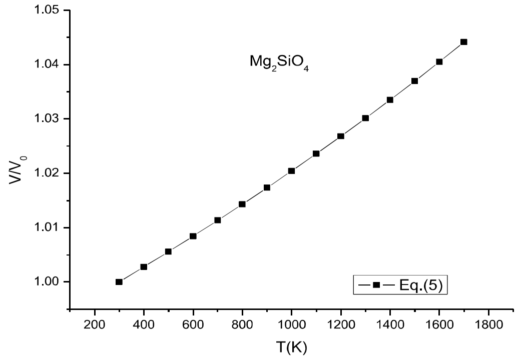

Fig.2-Temperature dependence of V/V_0

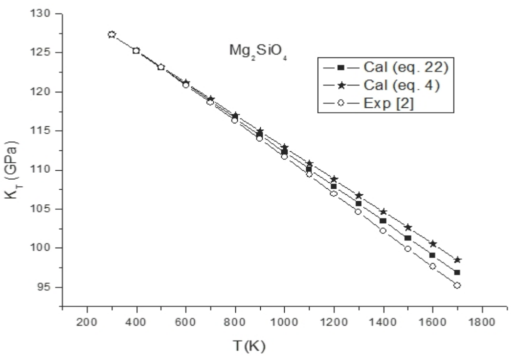

Fig.-3 Temperature dependence of K_T.

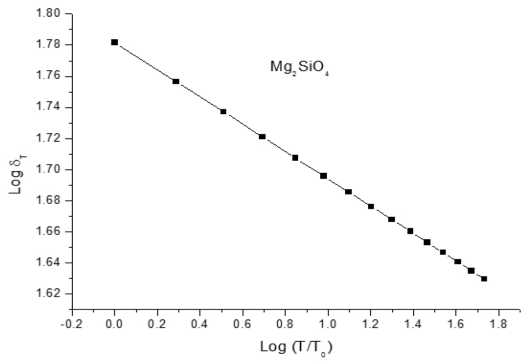

Fig.-4 Graph between $\log(T/T_0)$ vs $\log \delta_T$.

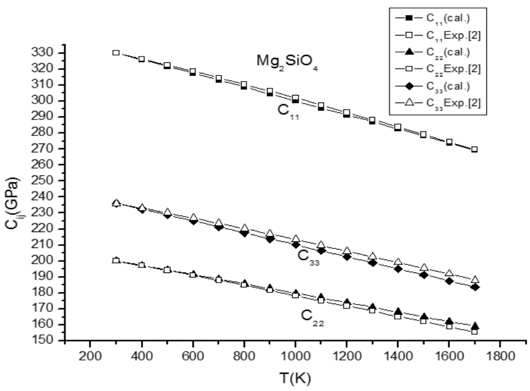

Fig.-5 Temperature dependence of C_{11}, C_{22} and C_{33}.

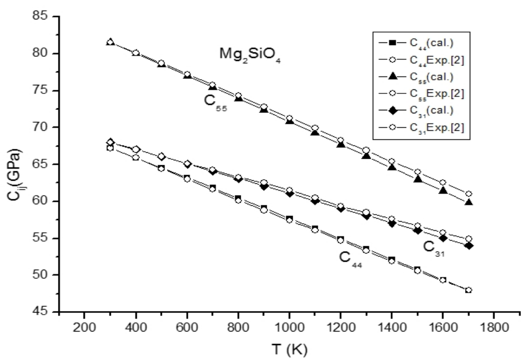

Fig.-6 Temperature dependence of C_{44}, C_{55} and C_{31}.

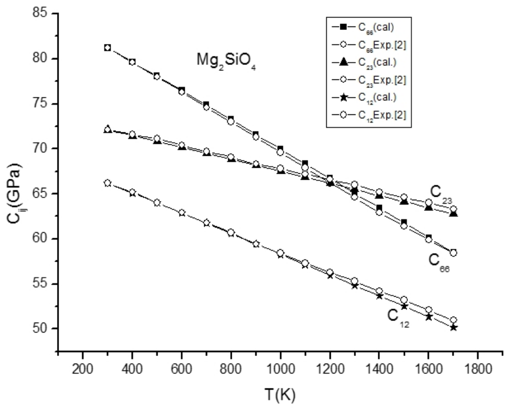

Fig.-7 Temperature dependence of C_{66}, C_{23} and C_{12}.

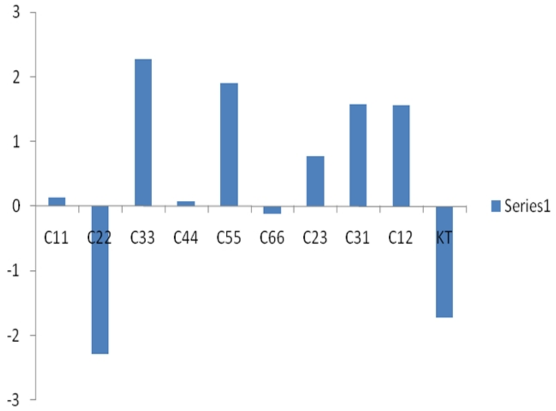

Fig.- 8 Percentage deviations at T = 1800K using eq. (25) with experimental data

We have thus presented a simple and straightforward method, to study the thermophysical and thermoelastic properties of Mg_2SiO_4 under varying conditions of temperature. The results obtained are demonstrated and encouraging that the present method is far better as compared with earlier studies[18-20].Due to the simplicity of the method, it can be extended to more complex solids like minerals of geophysical importance and applications.

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