Temperature Reliance of Elastic Constants for Two Geophysical Minerals

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Abstract : *- In the present paper, we developed relationship to predict temperature dependence of elastic constants for geophysical minerals by using a formulation for volume dependence of isothermal Anderson- Grünesien parameter which is valid upto extreme compression limit $P \rightarrow \infty$ or $V \rightarrow 0$. The present relationship are applied on geophysical minerals viz. MgO and CaO to validate the present expressions. We find that the calculated results of elastic constants are in good agreement with the experimental data. A close agreement between results and experimental data discloses the validity of present work.*

Keywords: - Elastic properties, Thermodynamic properties, Elastic Constants, Geophysical minerals.

1.0 Introduction

The knowledge of temperature dependence of elastic constants is very important to understand the thermo elastic behaviour of materials at high temperatures by many researchers [1-11]. The elastic constants explore the basic knowledge of Earth's deep interior [2]. Since the elasticity offers more information than the volume in interpreting the temperature dependence of Equation of State (EoS). There is still no general theory to calculate elasticity. The behaviours of elastic constants under the influence of high temperature have attracted the attention of experimental [8, 12] as well as theoretical workers [5-8]. Some phenomenological, semi phenomenological and empirical formulations have been developed to understand the change in elastic constants with the change in temperature at atmospheric pressure [9, 12]. The experimental data for temperature dependence of thermodynamic and elastic parameters for many solids have been compiled by Anderson [2, 3] which are considered to be most precise.

Thermal pressure is having an important role to study the thermodynamic and thermo elastic properties of solids. For understanding the adequacy of pressure-volume-temperature

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relationships, we need isothermal as well as isobaric equation of state (EoS). Anderson [2] scripted the EoS in terms of thermal pressure as follows:

$$P(V,T) = P(V,T_0) + \Delta P_{th} \quad (1)$$

where $P(V,T_0)$ constitutes the isothermal pressure-volume relationship at $T = T_0$,the inital temperature. ΔP_{th} is the pressure difference in the values of thermal pressure at two temperatures, i.e.

$$\Delta P_{th} = P_{th}(T) - P_{th}(T_0) \quad (2)$$

The following relationship between thermal pressure and thermal energy is

$$\Delta P_{th} = \rho\gamma E_{th} \quad (3)$$

where ρ is density and γ is the Grünesien parameter. In the present study, we generalised the volume dependence of Anderson - Grünesien parameter expression and for predicting values of temperature dependence of elastic constants of geophysical minerals MgO and CaO.

Method of analysis

2.0 Temperature dependence of elastic constants

Thermal expansivity is defined as [2]

$$\alpha = \frac{1}{V}\left(\frac{\partial V}{\partial T}\right)_P \quad (4)$$

The isothermal Anderson - Grünesien parameter (δ_T) is an important quantity to estimate the elastic properties of solids at high temperatures and pressures, which is defined as [1]

$$\delta_T = -\frac{1}{\alpha K_T}\left(\frac{\partial K_T}{\partial T}\right)_P \quad (5)$$

where α and K_T are known as thermal expansivity and isothermal bulk modulus respectively. Many researchers [6-8] have shown the various forms for the volume dependence of δ_T. Various workers [2,9] pointed out the similarity for volume dependence of γ and δ_T. We therefore generalize the relationships for volume dependence of Anderson – Grünesien parameter as follows

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$$\delta_T = \delta_{T_\infty} + (\delta_{T_0} - \delta_{T_\infty})\left(\frac{V}{V_0}\right)^{K_0'} \quad (6)$$

where δ_{T_0} and δ_{T_∞} are the values of δ_T at zero pressure and infinite pressure respectively. According to extreme compression or pressure thermodynamics Anderson- Grünesien parameter remains positive finite at infinite pressure i.e., $P \to \infty$ *or* $V \to 0$.

By using Eq. (4) & (5), we get the following relationship

$$\delta_T = -\frac{V}{K_T}\left(\frac{\partial K_T}{\partial V}\right)_P \quad (7)$$

Inserting Eq. (6) in Eq. (7), we get the following relationship

$$\frac{K_T}{K_0} = \left(\frac{V}{V_0}\right)^{-\delta_{T\infty}} exp\left\{\frac{\delta_{T0} - \delta_{T\infty}}{K_0'}\left(1 - \frac{V}{V_0}\right)^{K_0'}\right\} \quad (8)$$

Eq. (8) can also be modified to express the adiabatic bulk modulus (Ks) with volume expansion ratio as

$$\frac{K_S}{K_0} = \left(\frac{V}{V_0}\right)^{-\delta_{S\infty}} exp\left\{\frac{\delta_{S0} - \delta_{S\infty}}{K_0'}\left(1 - \frac{V}{V_0}\right)^{K_0'}\right\} \quad (9)$$

where δ_s is adiabatic Anderson Grünesien parameter which is defined as

$$\delta_S = -\frac{V}{K_S}\left(\frac{\partial K_S}{\partial V}\right)_P \quad (10)$$

where δ_{S_0} and δ_{S_∞} are the values of δ_S at zero pressure and infinite pressure respectively. It should be noted that $K'_{T\infty} = K'_{S\infty} = K'_\infty$ but $\delta_{T_\infty} \neq \delta_{S_\infty}$ [9]. Such fact can be understood by following thermodynamic identities [8, 9].

$$\delta_T = K_T' - 1 + q + C_T' \quad (11)$$

and

$$\delta_S = K_S' - 1 + q - \gamma - C_S' \quad (12)$$

where K_S' *and* K_T' are known as the first pressure derivative of bulk modulus at constant entropy and temperature respectively. Parameter q is known as the logarithmic volume derivative of γ or second Grünesien ratio, which tends to zero at infinite pressure. Terms C_S' *and* C_T' are related to the specific heat at constant volume and defined by following expressions

$$C_S' = \left(\frac{\partial ln\, C_V}{\partial lnV}\right)_S \quad (13)$$

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$$C_T' = \left(\frac{\partial ln\, C_V}{\partial lnV}\right)_T \tag{14}$$

The numerical values of C_S' and C_T' are very low and can be assumed to be zero, especially, at high pressure or at high temperature [9]. It is necessary to mention here that the temperature of solid increases as the applied pressure increases. At infinite pressure, Eqs. (11) and Eq. (12) are reduced to

$$\delta_{T_\infty} = (K_\infty' - 1) \tag{15}$$

and

$$\delta_{S_\infty} = (K_\infty' - 1) - \gamma_\infty \tag{16}$$

Again, according to Stacey and Davis [13], at infinite pressure the Slater's formula for the Grünesien parameter assumes the status of an identity, i.e.,

$$\gamma_\infty = \frac{1}{2} K_\infty' - \frac{1}{6} \tag{17}$$

Hence Eqs. (15)- (17) result following inter-relationship between δ_{T_∞} and δ_{S_∞}

$$2\delta_{S_\infty} = \delta_{T_\infty} - \frac{2}{3} \tag{18}$$

Thus the infinite pressure value of $\delta_T > \delta_S$. Relationship (15) provides a way to compute the value of δ_{T_∞} because K_∞' can also be computed by following empirical relationship [2]

$$K_\infty' = \frac{3}{5} K_0' \tag{19}$$

where K_0' the value of first pressure derivative of bulk modulus at ambient conditions. We generalize Eq. (8) in the following manner, by using the method of generalization [11].

$$\frac{C_{ij}}{C_{ij\,0}} = \left(\frac{V}{V_0}\right)^{-\delta_\infty} \exp \frac{\delta_{ij\,0} - \delta_{T\infty}}{K_0'} \left[1 - \left(\frac{V}{V_0}\right)^{K_0'}\right] \tag{20}$$

where C_{ij} is a value of elastic constant and its room temperature value is $C_{ij\,0}$, Here it is assumed that $\delta_{T\infty}$ remains constant for all elastic constants except K_S.

The $\delta_{ij\,0}$ is the value of an associated Anderson-Grünesien parameter ($\delta_{ij\,0}$) at zero pressure, which is defined as

$$\delta_{ij} = -\frac{1}{\alpha C_{ij}} \left(\frac{\partial C_{ij}}{\partial T}\right)_P \tag{21}$$

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3.0 Results and Discussions

Input parameters used in the calculations are cited in Table 1. We investigated the temperature dependence of isothermal bulk modulus and adiabatic bulk modulus. With the help of Eq. (8) and Eq. (9), we find the value of K_T and K_S for geophysical minerals viz. MgO and CaO. The value of δ_{T_∞} and δ_{S_∞} are estimated from Eqs. (15) to Eq.(19). Values of density (ρ), volume expansion ratio $\left(\frac{V}{V_0}\right)$ and Grünesien parameter (γ) have been taken from Anderson [2] to calculate K_T and K_S for geophysical minerals in Table 1. Predicted values of K_T and K_S at P = 0 are compared in Figures 1 to 4 with available experimental data compiled by Anderson and Issak [33]. Eq. (20) is used to calculate C_{11}, C_{44}, C_s for MgO, CaO. Computed values through Eq. (20) are also shown in Figures 1 to 4 available with experimental data [2].

4.0 Conclusions

It is concluded that we developed new expressions for temperature dependence of elastic constants on the basis of generalisation for the volume dependence of Anderson-Grünesien parameter at atmospheric pressure i.e., P = 0. These expression are used to compute elastic module such as K_S, K_T, C_{11}, C_{44} and Cs for geophysical minerals viz. MgO and CaO. A close agreement between the present approach and experiment reveals the validity of the present approximation. The results obtained from the present relationship shows the reliability with the generalised data based on the experimental data K_S, K_T, C_{11}, C_{44} and Cs.

Table -1 Values of input parameters used in calculations

Elastic constants		MgO	CaO
C^0_{ij} (GPa) [2]	C_{11}	299	330
	C_{44}	157.1	67.2
	C_S	101.3	—
	K_S	163.9	—
	K_T	161.6	—
δ^0_{ij}[1] [2]	C_{11}	5.45	3.78

	C_{44}	2.51	6.3
	C_S	8.77	—
	K_S	3.19	—
	K_T	4.92	—
K'_0 [1]		4.15	5.4

MgO				CaO			
T(K)	**V/V_0[2]**	**ρ[2]**	**γ [2]**	**T(K)**	**V/V_0[2]**	**ρ[2]**	**γ [2]**
300	1.000	3.585	1.54	300	1.000	3.349	1.35
400	1.003	3.573	1.53	400	1.003	3.338	1.36
500	1.007	3.559	1.53	500	1.007	3.327	1.37
600	1.011	3.545	1.54	600	1.011	3.314	1.37
700	1.015	3.531	1.53	700	1.015	3.301	1.37
800	1.020	3.516	1.53	800	1.019	3.288	1.37
900	1.024	3.501	1.54	900	1.023	3.275	1.36
1000	1.028	3.486	1.54	1000	1.027	3.262	1.36
1100	1.033	3.470	1.53	1100	1.031	3.248	1.35
1200	1.038	3.454	1.53	1200	1.036	3.234	1.35
1300	1.043	3.438	1.52				
1400	1.048	3.422	1.52				
1500	1.053	3.405	1.52				
1600	1.058	3.388	1.51				
1700	1.064	3.371	1.5				
1800	1.069	3.354	1.5				

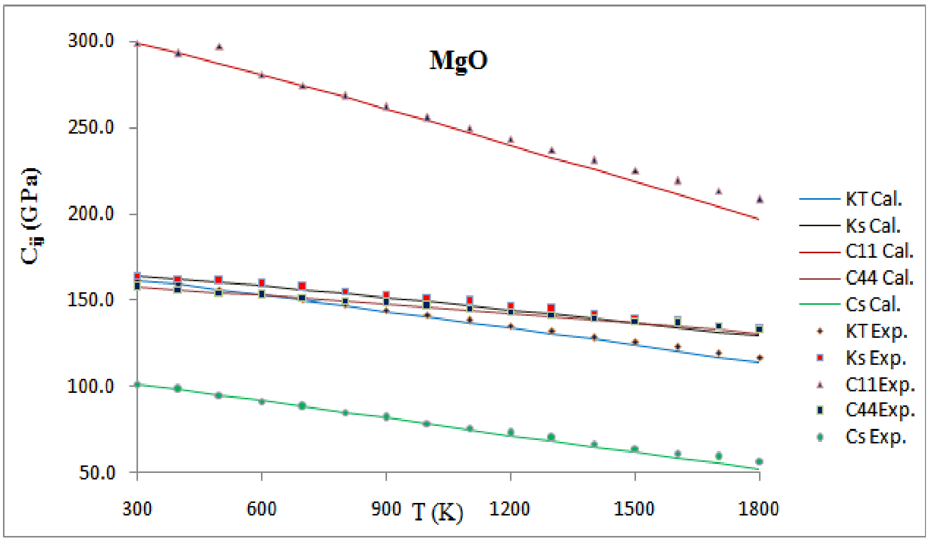

Fig. 1 Temperature dependence of elastic constants for MgO

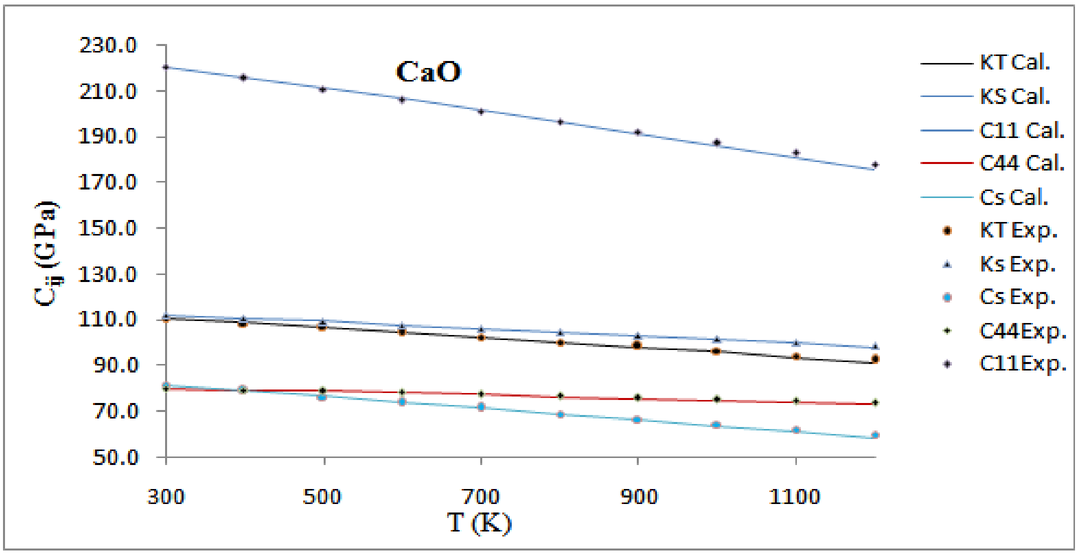

Fig. 2 Temperature dependence of elastic constants for CaO

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