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ELASTIC PROPERTIES OF PROTOTYPE SOLIDS UNDER HIGH TEMPERATURE

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ABSTRACT

We have formulated an expression for the temperature dependence of thermoelastic constants using the thermodynamic identities. It is found that all elastic moduli decreased with increasing temperature. Thus computed results using the present models show a better agreement with available experimental results. It is concluded that new expressions can also predict the elastic behavior of the Earth's minerals under high-temperature conditions and are used in geophysical applications.

Keywords: *Prototype Solids; Elastic Moduli; High Temperature.*

INTRODUCTION

Understanding the state of the earth's interior minerals and their density distribution under high pressure and high temperature attracts an increasing goal of researchers more than before [1]. Mineral physics has led the way in understanding the physical properties of matter under extreme conditions of pressure and temperature and the results of this research have been a significant impact in fields such as geophysics, materials science and condensed matter physics. The Elastic moduli are very important quantities to describe the mechanical properties of materials. They are evidently and directly employed to evaluate the elastic strains or energies in materials under the stress of various origins: external, internal, thermal, etc. Because elastic properties are also closely associated with many fundamental physical parameters, such as seismic velocities, anisotropy, Cauchy's deviation, thermal conductivity, Debye temperature, interatomic potentials, etc. The behaviors of elastic moduli under the effect of high temperature have widely attracted the attention of experimental [1-5] as well as theoretical researchers [6-23].

In the third paper, we will be derived the expression for the temperature dependence of elastic moduli using the basic thermodynamics relations [1, 5]. The derived expressions have been applied to some important prototype solids viz. MgO, CaO, NaCl, and KCl use to test the validity and applicability of the present study to evaluate the elastic properties under extreme temperatures.

The study of alkaline earth oxides (AEOs) is of great interest for several reasons because of these oxides i.e. MgO, and CaO have long been considered a typical case for understanding bonding in ionic oxides [22] and are also one of the most fundamental materials for industrial science. These oxides are also a major constituent of the earth's lower mantle (between 600 and 2900km in depth) [4]. The electronic structure [23], structural phase transitions [6-10], elasticity [1-20], thermal properties [1-3, 8-10], stability and the equation of state [12-16] of these oxides have been extensively studied theoretically [6-20] as well as experimentally [1-5].

Alkali halides have the first materials of choice in several experiments and are used in many experiments such as Laue experiments on X-ray diffraction and NaCl was one of the crystals which Bragg chose for structural analysis, experiment on thermal expansion of various crystals [24-25], and measurement of compressibility [26]. Alkali halides are convenient systems for scaling of properties. The lattice constant has been used to scale a large number

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of properties like elastic constants [27-28], Debye's theory of specific heat [29-30], and hardness, color centre parameters like concentration of defects [31]. Pure alkali halides are less stable and have poor mechanical strength. These limitations can be overcome by mixing and adding impurities in them. Because of it is suitably found to be useful and necessary to grow and characterize ternary crystals of various compositions [32-33].

The results from the proposed study have been discussed and a comparison made with the available experimental data. The present proposed work based on the equation of states under the extreme condition of temperature is very essential because of the fact that it allows the extrapolation into the regions for which the experimental data are not available abundantly.

Theoretical Analysis for Temperature dependence Elastic Constants:

In this section we will developed the expression for temperature dependence of elastic moduli using the Tallon's method [34]. Anderson et al [5] represent the expression for variation of thermal expansivity with change in temperature and given as follow:

$$\alpha/\alpha_0 = 1/[1 - \alpha_0\delta_T(T - T_0)] \quad \text{---------- (1)}$$

Where the subscript zero refers beginning point as usual meaning. Eq. (1) is applicable for extrapolations of the values α above the Debye temperature for perovskite. Here δ_T be the Anderson-Gruneisen parameter and it is independent of temperature.

The expansion of eq. (1) is truncated up to the third terms, δ_T replace by δ_{T0} and using the definition of thermal expansivity $\alpha = 1/V\left(\frac{\partial V}{\partial T}\right)_P$ and integrating. Thus, we can derived the expression for volume compression as follow

$$\frac{V_0}{V} = exp\left[\alpha_0\left\{(T - T_0) + \frac{1}{2}\alpha_0\delta_{T0}(T - T_0)^2 + \frac{1}{3}\alpha_0^2\delta_{T0}^2(T - T_0)^3\right\}\right] \quad \text{---------- (2)}$$

By the definition of isothermal Anderson-Gruneisen δ_T [5]

$$\delta_T = -\frac{1}{\alpha K}\left(\frac{\partial K}{\partial T}\right)_P \quad \text{---------- (3)}$$

Using eq. (2), eq. (3), replacingδ_T replace by δ_{T0} because of δ_T be the independent of temperature and integrating, thus we can easily determined the expression for temperature dependence bulk modulus and can be written as

$$K = K_o exp\left[-\alpha_0\delta_{T0}(T - T_0)\left\{1 + \frac{1}{2}\alpha_0\delta_{T0}(T - T_0) + \frac{1}{3}\alpha_0^2\delta_{T0}^2(T - T_0)^2\right\}\right] \quad \text{---------- (4)}$$

The eq. (4) may be used to determine the temperature dependence of elastic moduli by using the generalization method of Tallon [34] and the derived expression has become the same as reported in the previous study [12-16] yet the method of derivation is different than previous[16].

The relevant expression for elastic constants can be written collectively as follows:

$$M = M_o exp\left[-\alpha_0\delta_{ij0}(T - T_0)\left\{1 + \frac{1}{2}\alpha_0\delta_{ij0}(T - T_0) + \frac{1}{3}\alpha_0^2\delta_{ij0}^2(T - T_0)^2\right\}\right] \quad \text{---------- (5)}$$

Where M (C_{ij}, K, G) is the elastic moduli; M_0 (C_{ij0}, K_0, G_0) is the elastic moduli at ambient pressure and standard temperature may be 300K. Here δ_{ij0} is given by eq. (3) as defined by many authors [12-16, 35-37]. C_{ijo} and $C_{ij}^{\prime T}$ be the elastic constant and its temperature derivatives were used to determined the values of $\delta_{ij0} = -\frac{1}{\alpha_0 C_{ij0}}\left(\frac{\partial C_{ij}}{\partial T}\right)_0 = -\frac{C_{ij}^{\prime T}}{\alpha_0 C_{ij0}}$ at ambient conditions.

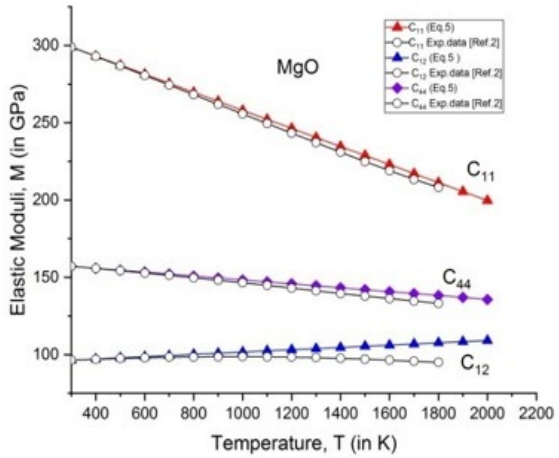
RESULTS AND DISCUSSIONS

The results obtained for four important prototype solids viz. MgO, CaO, NaCl, and KCl have been plotted in graphs. To check the validity of proposed work, we have compared our results with available experimental results. For this propose, the used fitting parameters have been shown in Table-1.

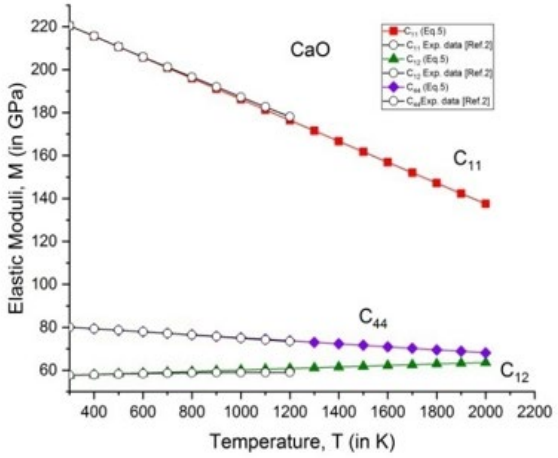
Table-1: Used input parameters Bulk moduli (M_{ij}) (in GPa), temperature derivative of elastic moduli ($M_{ij}^{\prime T}$) (in 10^{-2} GPa K^{-1}), coefficient of volume thermal expansion (α_0) (in 10^{-5} K^{-1}) and Isothermal Anderson-Gruneisen papameter (δ_{T0}) (dimensionless) at ambient pressure ($P = 0$) and room temperature (300 K).

Minerals	Moduli	C_{11}	C_{12}	C_{44}	K_T/K	G_0	Source
MgO $\alpha_0 = 3.12$ δ_{T0}= 5.3	M_{ij}	299	96.4	57.1	161.6	131.8	Ref.[2]
	$M_{ij}^{\prime T}$	-5.85	0.75	1.26	-	-	Ref.[38]
CaO $\alpha_0 = 3.04$ δ_{T0}= 6.19	M_{ij}	220.5	57.67	80.03	110.6	80.59	Ref.[2]
	$M_{ij}^{\prime T}$	-4.90	0.35	-0.70	-	-	Ref.[38]
NaCl $\alpha_0 = 11.8$ δ_{T0}= 5.56	M_{ij}	49.5	13.2	12.79	24.0	14.71	Ref.[2]
	$M_{ij}^{\prime T}$	-3.67	-0.008	-0.354	-	-	Ref.[39]
KCl $\alpha_0 = 11.0$ δ_{T0}= 5.84	M_{ij}	40.1	6.6	6.35	17.0	9.47	Ref.[2]
	$M_{ij}^{\prime T}$	-3.30	0.24	-0.213	-	-	Ref.[39]

Using the input parameters shown in the Table.1, we have computed the results of temperature dependence elastic moduli for MgO, CaO, NaCl, and KCl using derived the eq. (4) and (5). We have analyzed temperature dependence elastic moduli with their explanations and compare with experimental results [2]. The obtained results have been plotted C_{ij} vs. temperature in fig.1 and K& G vs. temperature has shown in fig.2. The variation of second-order elastic constants with temperature has been shown in fig. 1(a-d) for MgO, CaO, NaCl, and KCl. It is clear from fig.1(a-d), the value of C_{11} sharply decreases with the increase of temperature, the value of C_{12} fewer increases with increasing temperature i.e appears as almost constants with increase with temperature. The value of C_{44} slowly decreases with the increase in temperature. The variation of bulk modulus and shear moduli with temperature has been shown in fig.2 (a-d) for MgO, CaO, NaCl, and KCl and both are a slightly less rapid decrease with the increase in temperature in comparison to C_{11}. We have therefore computed the percentage deviation at the highest temperature of the results obtained using the derived formulation with experimental results reported by Anderson and Isaak [2] and reported in Table-2. It has been found that the derived the eq. (4) and (5) gives good agreement with the experimental results reported by Anderson and Isaak [2] except in a few cases C_{12} for MgO, C_{11} and C_{44} for KCl.



(a) MgO



(b) CaO

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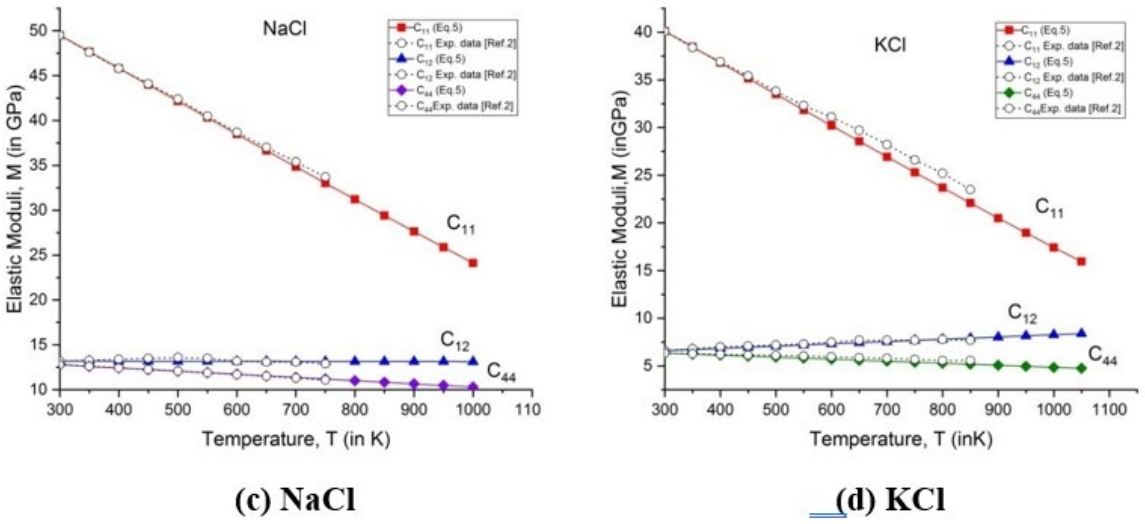
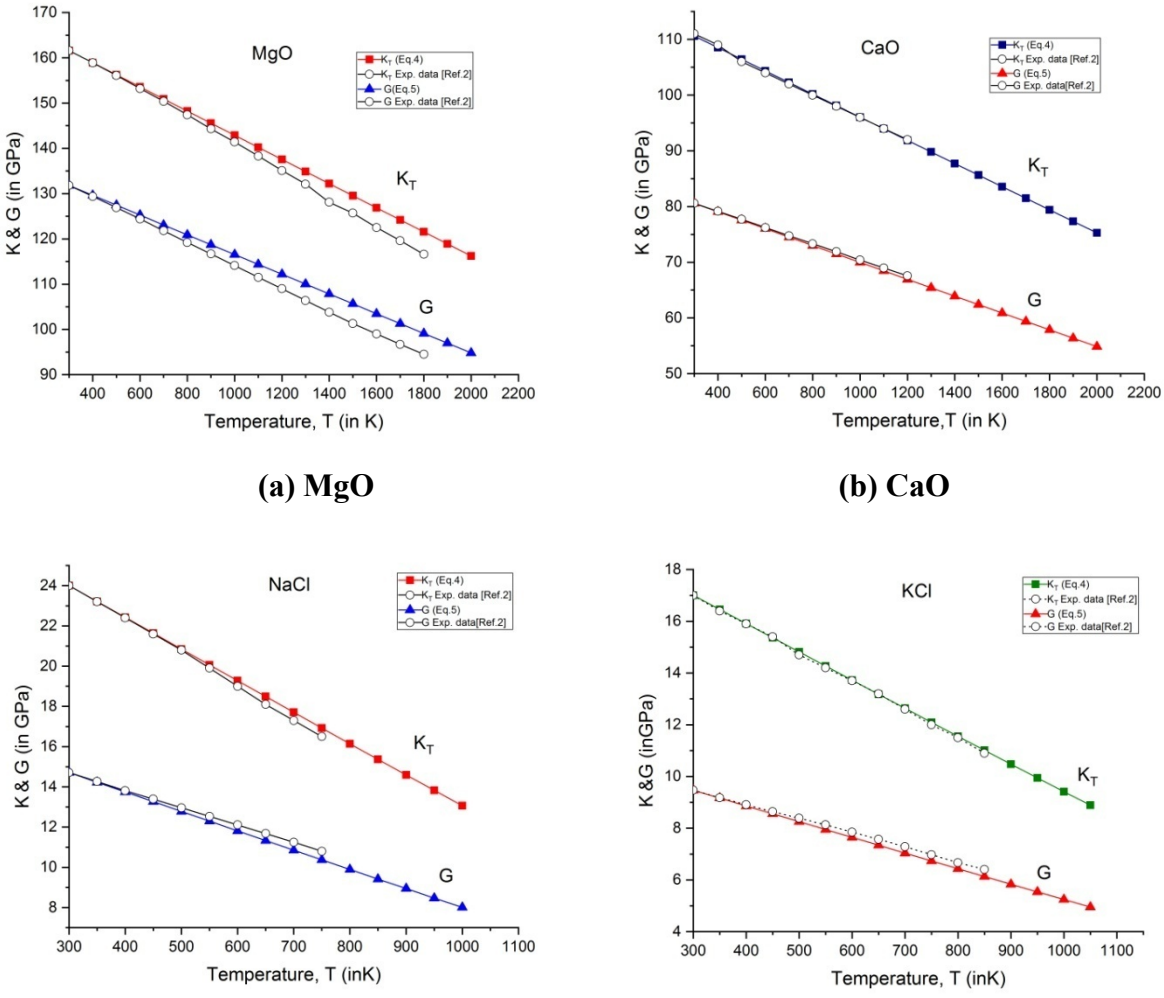


(c) NaCl **(d) KCl**

Fig 1. Temperature dependence of elastic moduli C_{ij} for (a) MgO; (b) CaO; (c) NaCl; (d) KCl. The filled symbols indicate the calculated results and open circle symbols show the experimental data [2].



(a) MgO **(b) CaO**

(c) NaCl **(d) KCl**

Fig 2. Temperature dependence of bulk modulus K and Shear Modulus $G$for (a) MgO; (b) CaO; (c) NaCl; (d) KCl. The filled symbols indicate the calculated results and open circle symbols show the experimental data [2].

Table-2: The percentage deviation at the highest temperature of the results obtained using the derived formulation with experimental results reported by Anderson and Isaak [2].

Highest Temperature	Minerals	C_{11}	C_{12}	C_{44}	K	G
1800 K	MgO	1.50	**13.34**	3.84	4.24	4.90
1200 K	CaO	0.95	3.10	0.34	0.14	0.91
750 K	NaCl	2.01	2.05	0.87	2.57	3.95
850 K	KCl	**6.02**	2.85	**7.02**	1.02	4.31

In general, the deviations are in C_{12}. The abnormal behavior of the temperature dependence of the elastic constant C_{12} is related to the existence of many body potential and non-central potentials in solids, which are responsible for the breakdown of Cauchy relation $C_{12} = C_{44}$ reported in previous literature [16, 35-37, 40]. The variation C_{11} represents the elasticity in length. A longitudinal strain produces a change in compression without change in shape. The volume change is closely related to the temperature and thus produces a large change in C_{11}. On the other hand, C_{12} and C_{44} are related to the elasticity in shape which is a shear constant. A transverse strain or shearing causes a change in shape without a change in volume [40-42]. Therefore, C_{12} and C_{44} are less sensitive to the temperature. Thus the study of the temperature dependence of C_{11} may provide the critical test of the present formulation.

Thus the derived formulation is capable to predict the elastic moduli under the varying conditions of temperatures. The obtained results are encouraging us to the straight forward methods of analysis. Due to the modesty of method, it can be implemented to other complicated minerals having geophysical importance and applications.

CONCLUSIONS

The obtained results from the proposed EOSs are very satisfactory in comparison to other theoretical models [5, 8-9]. The main features of these models are fewer input parameters are required which are easily available in various literatures. We have made an attempt to investigate the elastic properties of KCl under high pressure because of fewer works that have been reported in this case. These models may be frequently employed as the thermal equation of states of Earth's minerals using the various advanced quantum methods and simulations at the pressure and temperature of the earth's interior. The major achievement of these models is that follows the basic laws of thermodynamic with regard to expression at high-pressure and hence allows extrapolation to regions for which experimental data are not available. These models may, therefore, be useful for future planning high-pressure experiments on the compression behavior of the earth forming minerals, solids, nanomaterials, etc.

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