International Journal of Trend in Scientific Research and Development (IJTSRD)
Volume 4 Issue 4, June 2020 Available Online: www.ijtsrd.com e-ISSN: 2456 – 6470

Pressure Derivatives of Bulk Modulus, Thermal Expansivity and Grüneisen Parameter for MgO at High Temperatures and High Pressures

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ABSTRACT

Expression for the Bulk modulus and its Pressure derivatives have been derived and reduced to the limit of infinite pressure. The Pressure dependence of thermal expensively and the Grüneisen Parameter both are determined using the formulations which satisfy the thermodynamic constraints at infinite pressure. Values of Bulk modulus and its Pressure derivative are also obtained for the entire range of Temperatures and Pressures considered in the present study. We have also investigated the Thermo elastic Properties of MgO at high Temperature and High Pressures using the results based on the EOS. The method based on the calculus in determinates for demonstrating that on the physically acceptable EOS Satisfy the identities for the pressure derivatives of bulk modulus Materials.

KEYWORDS: *Pressure derivatives, Bulk modulus, Thermal Expansively, Grüneisen Parameter, MgO, Infinite Pressure behavior*

How to cite this paper: Dr. Sheelendra Kumar "Pressure Derivatives of Bulk Modulus, Thermal Expansivity and Grüneisen Parameter for MgO at High Temperatures and High Pressures" Published in International Journal of Trend in Scientific Research and Development (ijtsrd), ISSN: 2456-6470, Volume-4 | Issue-4, June 2020, pp.1440-1442, URL: www.ijtsrd.com/papers/ijtsrd31614.pdf

IJTSRD31614

INTRODUCTION:

For investigating high pressure properties of materials, we need equations of state representing the relationships between pressure P and volume V at a given temperature T [1,2] in the range 300K to 3000K using the Stacey reciprocal **K**-Primed EOS[3]. Some important equations of state such as the Birch-Murnaghan finite strain equation [4], the Poirier-Tarantula logarithmic equation [5,] the Keane K-primed equation[6] Have been widely used for Various materials. MgO is an Important and ceramic and Geophysical mineral [1,7,8] with various applications in the field of condensed matter physics and geophysics. It has large bulk modulus, less compressibility and high melting temperature [9, 10]. MgO remains stable in the rock salt (NaCl) Structure starting from the room temperature up to the melting temperature and up to a pressure of nearly 225 GPa. The melting temperature more than 3000K for MgO is nearly three times larger than is Debay temperature nearly equal to 1000K. Also the phase transition pressure for MgO is much higher pressure then its bulk modules value of temperature and pressure for MgO to investigate its thermo elastic properties [11,12]. Values of K and its pressure derivatives $K' = dK/dP$ have also been calculated for the entire range of P and T. The result for P, K and K' obtained from the Stacey equation are used to determine the thermal expansively and The Grüneisen parameter with help of the formulations which satisfy the boundary conditions at infinite pressure. The Grüneisen parameter γ is an important physical quantity directly related to thermal and elastic properties of materials [1, 2, 13] as follows.

$$\gamma = \frac{\alpha K_T V}{C_V} = \frac{\alpha K_S V}{C_P} \qquad (1)$$

Where α is the thermal expansivity, K_T and K_S are isothermal and adiabatic bulk module, C_v and C_p are specific heats at constant volume and constant pressure, respectively. Its is worth mentioning here that various physical quantities appearing in Eq.(1) differ much from one materials to the other , but γ remains nearly about 1.5 for a wide range of materials.

Method of analysis:

All of these equations reveal the pressure P and bulk models K both increase rapidly with the decreasing volume. P and K both become infinite in the limit of extreme compression (V→0), but their ratio remains finite such that :

$$\left(\frac{P}{K}\right)_\infty = \frac{1}{K'_\infty} \qquad (2)$$

where K'_∞ is the value of $K' = \frac{dK}{dP}$, the pressure derivative of bulk modulus at infinite pressure. It should be mentioned that K' represents the role of increase of bulk modulus with the increase in pressure. The Brich –Murnaghan EOS , the Poirier-Tarantola logarithmic EOS , and the generalized Rydberg- Vinet EOS, all can be represented by the following common formula:

$$\frac{K}{P} = K'_{\infty} + f(x) \quad (3)$$

Where f(x) is a function of x= V/V_0 V_0 is the value of volume V at P=0 of K' and f(x) are different for different EOS. Thus for the Birch-Murnaghan fourth order EOS, K'= 11/3, and

The Stacey reciprocal K-primed equation of state is wriiten as follows [3]

$$\frac{1}{K'} = \frac{1}{K'_0} + \left(1 + \frac{K'_{\infty}}{K'_0}\right)\frac{P}{K} \quad (4)$$

Equation (4) represents a linear relationship between 1/K' and P/K such that [14].

$$\frac{1}{K'_{\infty}} = \left(\frac{P}{K}\right)_{\infty} \quad (5)$$

The subscripts 0 and ∞ represent values at zero - pressure and at infinite pressure, respectively. Eq. (4) has been integrated analytically [10, 11] to find

$$\frac{K}{K_0} = \left(1 - K'_{\infty}\frac{P}{K}\right)^{-\frac{K'_0}{K'_{\infty}}} \quad (6)$$

Eq. (6) has also been integrated to yield [8, 10]

$$\ln\frac{V}{V_0} = \frac{K'_0}{K'^2_{\infty}} In\left(1 - K'_{\infty}\frac{P}{K}\right) + \left(\frac{K'_0}{K'_{\infty}} - 1\right)\frac{P}{K} \quad (7)$$

For determining values of thermal expansivity α at different pressure along elected isotherm we use the formulation [12] which satisfies the thermodynamics constraints [10] according to which the thermal expansivity vanishes in the limit of infinite pressure. Values of Grüneisen parameter γ relationship recently formulated by shanker at al. [13]. This formulation yields satisfactory results for the Earth lower , mantel and core in good agreement with the seismic data [10].

The formulation used for α (P) is written as follows [12]

$$\alpha = \alpha_0\,(1\text{-}K'P/K)^{t} \quad (8)$$

where α_0 is the thermal expansivity α at zero pressure. t is a material dependent constant. We have calculated values of α using Eq.(8) which is consistent with the thermodynamic constraints that α tends to zero in the limit pressure [2,13] Eq. (5) at infinite pressure when used in Eq. (8) gives α equal zero.

The reciprocal gamma relationship can be written as follows

$$\frac{1}{\gamma} = \frac{1}{\gamma_0} + K'_{\infty}\left(\frac{1}{\gamma_{\infty}} - \frac{1}{\gamma_0}\right)\frac{P}{K} \quad (9)$$

Where γ_0 and γ_{∞} are respectively the values of γ at zero pressure in the limit of infinite pressure.\

Result and Discussions

It should be emphasized that the pressure derivatives of bulk modulus are of central importance for determining thermoplastic properties of materials lat high pressure and high temperatures. The formulation presented here is related to different equations of state which have been used recently for investigating properties of materials at high pressure. for investigating the pressure-volume relationship at high temperatures , the thermal pressure is of central importance [1, 15, 16]. We can determine thermal pressure by lowing the values of thermal expensivity and bulk modulus at high temperatures [7,8,14] An alternative method for determining pressure-volume relationship at higher temperatures has been developed [7,8,15] using phenomenological equation of state with temperatures dependent values of input parameters K_0 and K'_0. For MgO,

Conclusions:

We have used the Stacey reciprocal K-primed equation of state which satisfies important boundary conditions at infinite pressure .It is found from the P-V-T results obtained for MgO that for producing the same amount of compression $\left(\frac{V}{V_0}\right)$. Values of bulk modulus K increase with the increase with the increase in pressure, and decrease with the increase in temperature. Since the bulk modulus is inverse of compressibility, it becomes harder to compress the solid at higher pressures because of the increasing bulk modulus. One of the most important thermodynamic constraints due to Stacey [13] is the fact that thermal expansivity of a material vanishes in the limit infinite pressure the reciprocal gamma equation has been shown to be compatible with the Stacey reciprocal K-primed equation both.

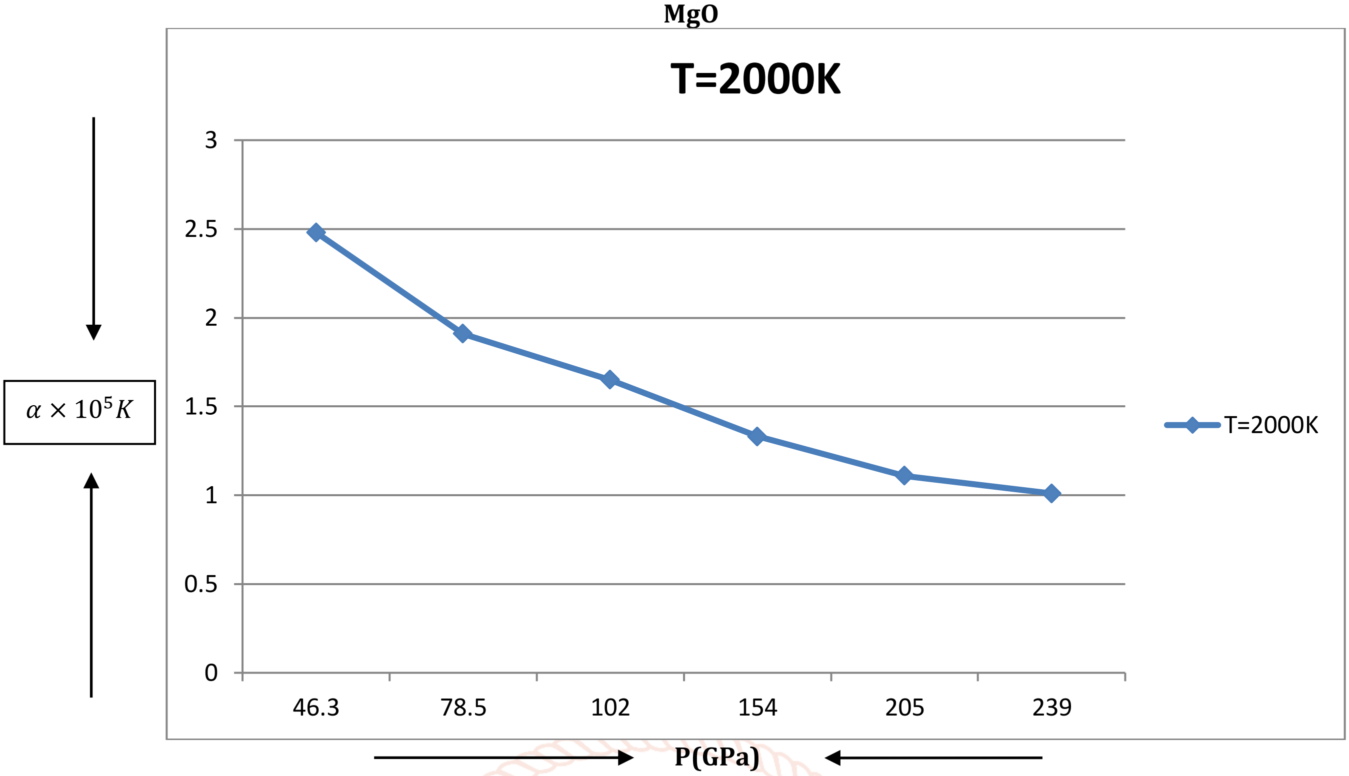
The equation yield similar expression for the higher order derivatives at infinite pressure. We may thus conclude that status of an identity which can be used for determining the third order Grüneisen Parameter [17].

Acknowledgements:

We are thankful to the reviewers for their helpful comments. Thanks are also due to Professor Anuj Vijay & Professor J. Shanker, for some very useful discussions.

P(GPa)	0.00	46.30	102	154	205	239
α at T=2000K	5.48	2.48	1.65	1.23	1.11	0.941

MgO



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