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

The Grüneisen Parameter and Higher Order Thermo Elastic Properties of Fe, Co at Higher Pressures

Dr. Sheelendra Kumar

Assistant Professor, Department of Physics, C.C.S.P.G. College Heonra, Uttar Pradesh, India

ABSTRACT
Expressions have been obtained for the higher order Thermo elastic properties of the Grüneisen parameter in the limit of infinite pressure The usefulness of these expressions has been demonstrated by considering a relationship between reciprocal Grüneisen parameter and the pressure bulk modulus ratio at finite pressure. The results have been obtained using the shanker reciprocal gamma relationship. The results have also been determined using the Stacey-Davis formulations for the third order Grüneisen parameters. The calculations have been performed in case of transition metals Fe & Co for the wide range of compressions. It has been found that both the models yield close agreement with each other. The obtained results in the present paper satisfy the thermodynamic constraints in the limit of infinite pressure.

KEYWORDS: Grüneisen parameters, Thermoelastic properties, infinite pressure behavior, transition metal

How to cite this paper: Dr. Sheelendra Kumar "The Grüneisen Parameter and Higher Order Thermo Elastic Properties of Fe, Co at Higher Pressures" Published in International Journal of Trend in Scientific Research and Development (ijtsrd), ISSN: 2456-6470, Volume-4 | Issue-4, June 2020, pp.994-996, URL: www.ijtsrd.com/papers/ijtsrd31435.pdf

IJTSRD31435

INTRODUCTION
The Grüneisen parameter γ is related to Thermoelastic properties of materials [1-3]. The pressure derivatives of γ play a central role in predicting the thermal behavior , equation of state, and melting at high pressures [4-6]. The Grüneisen parameter γ is an important physical quantity directly related to thermal and elastic properties of materials [7–9] as follows

$$\gamma = \frac{\alpha K_T V}{C_V} = \frac{\alpha K_S V}{C_P} \tag{1}$$

Where α is the thermal expansivity K_T and K_S are isothermal and adiabatic bulk moduli, C_V and Cp are specific heats at constant volume and constant pressure, respectively. For a given material γ decreases with increasing pressure P or decreasing volume V.

There have been various attempts [7–11] to formulate expressions for γ(V) as well as γ(P). The most critical examination of these formulations can be made by applying the thermodynamic constraints for the higher–order Grüneisen parameters [7,9, 15–17] at extreme compression in the limit of infinite pressure. In the presented study, we have been determined the higher order Grüneisen parameter in case of transition metals Fe, Co for the wide range of compressions.

Formulation for γ(V):
According to the Stacey- Davis model we can write

$$\lambda = \lambda_\infty + (\lambda_0 - \lambda_\infty)\frac{q}{q_0} \tag{2}$$

On integrating Eq. (2), we get

$$q = q_0\left[1 + \frac{\lambda_0}{\lambda_\infty}\left(\frac{V_0}{V}\right)^{\lambda_\infty} - \frac{\lambda_0}{\lambda_\infty}\right]^{-1} \tag{3}$$

And further integration gives

$$\gamma = \gamma_0\left[\frac{\lambda_0}{\lambda_\infty} - \left(\frac{\lambda_0}{\lambda_\infty} - 1\right)\left(\frac{V_0}{V}\right)^{\lambda_\infty}\right]^{-\frac{q_0}{(\lambda_0 - \lambda_\infty)}} \tag{4}$$

It has been found [5,8] that if we assume

$$(\lambda_0 - \lambda_\infty) = q_0 \tag{5}$$

Eq. (13) 0n differentiation yields

$$\xi = \left(\frac{\lambda_0 - \lambda_\infty}{q_0}\right)q \tag{6}$$

In the present study we use Eq. (2), (3), (4) and (6) to obtain γ, q, λ and ξ for transition metals.

Formulation for γ(*P*)
The generalized free –volume formula for γ as a function of pressure *P*, bulk modulus and its pressure derivative *K'* = *dK* / *dP* has been widely used in literature [18–21]. This formula is written as follows [8–10]

$$\gamma = \frac{\frac{K}{2} - \frac{1}{6} - \frac{f}{3}\left(1 - \frac{P}{3K}\right)}{\left(1 - 2f\frac{P}{3K}\right)} \tag{7}$$

where *f* is the free –volume parameter. Different values of *f* such as 0, 1, 2 and 2.35 have been taken by Slater [18], Dugdale and MacDonald [19], Volume dependence of Grüneisen parameter 199

Vashchenko and Zubarev [20], and by Barton and Stacey [21]. The main difficulty associated with Eq. (7) is regarding the uncertainties in the value of f arising from various approximations involved in the derivation of the formula [9]. It is even more uncertain to use Eq. (7) for evaluating derivatives of γ because of difficulties in determining df / dP and $d2 f / dP2$. Such calculations are tedious at finite pressures. However, it should be indicating that Eq. (7) in the limit of infinite pressure gives expressions [9, 15] which are free from the free –volume parameter f. An alternative formulation for _(P) has been presented by Shankar et al. [17]. They proposed the following relationship

$$\frac{1}{\gamma} = \frac{1}{\gamma_0} + K_\infty^{\cdot}\left(\frac{1}{\gamma_\infty} - \frac{1}{\gamma_0}\right)\frac{P}{K} \tag{8}$$

Where $K_\infty$is the minimum value of $K^{\cdot}$ in the limit of infinite pressure. Eq. (8) satisfies the following identity [20, 3]

$$\left(\frac{P}{K}\right)_\infty = \frac{1}{K_\infty} \tag{9}$$

Eq. (8) yields the following expressions for the higher order derivatives of the Grüneisen parameter [16]

$$\frac{q}{\gamma} = K_\infty^{\cdot}\left(\frac{1}{\gamma_\infty} - \frac{1}{\gamma_0}\right)\left(1 - K^{\cdot}\frac{P}{K}\right) \tag{10}$$

$$\lambda = \frac{KK^{\cdot}}{(1-K^{\cdot}P/K)}\frac{P}{K} + K^{\cdot} + q \tag{11}$$

$$\xi = -\frac{2KK^{\cdot}}{\lambda\,(1-K^{\cdot}P/K)} - \frac{(K^{\cdot}KP/K)^2}{\lambda(1-K^{\cdot}P/K)^2} - \frac{K^2K^{\cdot}\left(\frac{P}{K}\right)}{\lambda(1-K^{\cdot}P/K)} + q \tag{12}$$

It should be mentioned that the expressions for γ, q, λ and ξ given above satisfy the boundary conditions in the limit of infinite pressure viz. γ_∞ and λ_∞ both remain positive finite whereas $q\infty$ and $x\infty$ both tend to zero. Equations (8), (10), (11) and (12) at infinite pressure become identical to the corresponding expressions derived from the basic principles of calculus which have the status of identities [13, 14, 16].

INFINITE PRESSURE BEHAVIOUR

P is a function of V such that increases continuously with the decreasing V. At extreme compression ($V \to 0$), P becomes infinitely large, then we can write

$$\left(\frac{dlnP}{dlnV}\right)_{V\to 0} = negative\ finite \tag{13}$$

Since

$$\frac{dlnP}{dlnV} = -\frac{K}{P} \tag{14}$$

Where K is bulk modulus

$$K = -V\frac{dP}{dV} \tag{15}$$

Eq. (13) and (14) yield

$$\left(\frac{K}{P}\right)_\infty = positive\ finite \tag{16}$$

Now taking $y = \frac{K}{P}\ and\ x = V$

in expression $\left(\frac{dlny}{dlnx}\right)_{x\to 0} = 0$

Where y is a function of x such that y remains positive finite at x→ 0

if y becomes zero at x→ 0

$$\left[\frac{dln(K/P)}{dlnV}\right]_{V\to 0} = 0 \tag{17}$$

Because K/P is positive finite (Eq. 16), on solving Eq. (17), we get

$$(1 - K^{\cdot}\,P/K)_\infty = 0 \tag{18}$$

Eq. (18) yields

$$K_\infty^{\cdot} = \left(\frac{K}{P}\right)_\infty \tag{19}$$

Equation (19) has the status of an identity [7,5, 20]. In view of Eq. (16), it is revealed from Eq. (19) that$K_\infty^{\cdot}$, the pressure derivative of bulk modulus, dK/dP, at infinite pressure remains positive finite.

Result and discussion

The quantities calculated as a function of pressure can be converted to those as a function of volume. and vice versa with the help of an equation of state theory. We use the Stacey K- primed equation of state [9] which is based on Eq.(9). And can be expressed as

$$\frac{1}{K} = \frac{1}{K_0} + \left(1 - \frac{K_\infty^{\cdot}}{K_0^{\cdot}}\right)\frac{P}{K} \tag{20}$$

On integration, Eq. (20) gives

$$\frac{K}{K_0} = \left(1 - K_\infty^{\cdot}\frac{P}{K}\right)^{-K_0^{\cdot}/K_\infty^{\cdot}} \tag{21}$$

Further integration of Eq. (21) gives

$$\ln\left(\frac{V}{V_0}\right) = \left(\frac{K_0^{\cdot}}{K_\infty^{\cdot}} - 1\right)\left(\frac{P}{K}\right) + \frac{K_0^{\cdot}}{K_\infty^{\cdot 2}}\ln\left(1 - K_\infty^{\cdot}\frac{P}{K}\right) \tag{22}$$

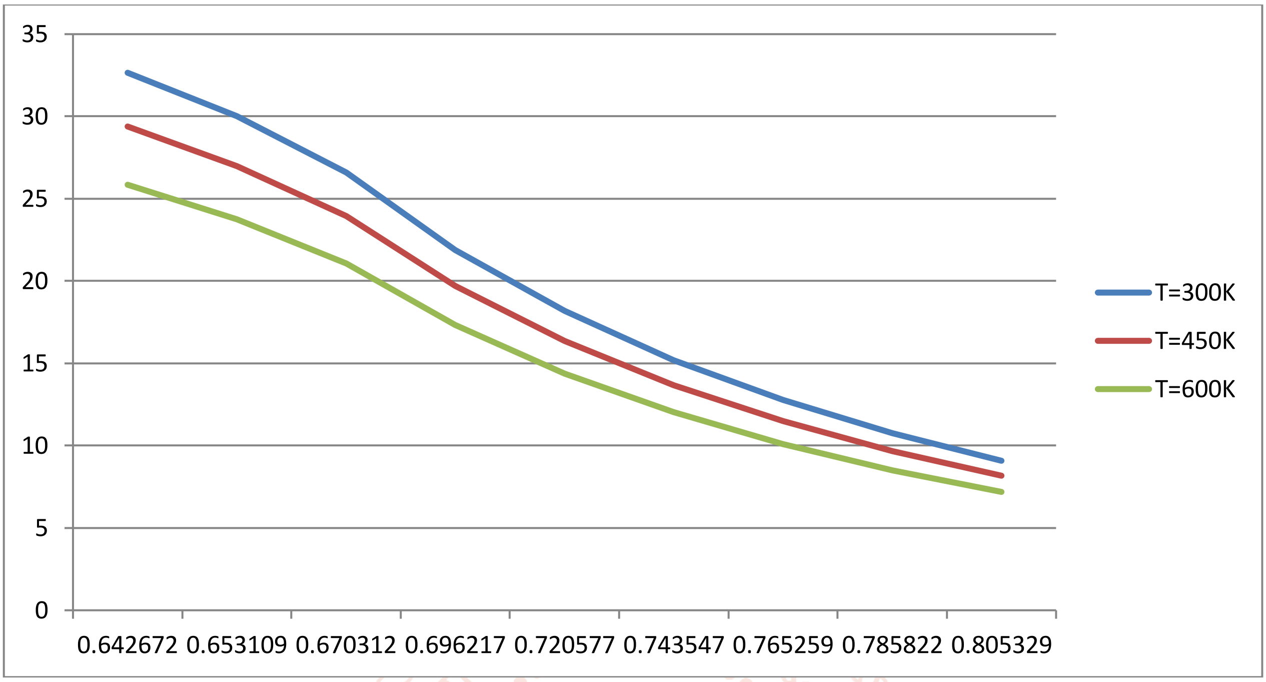
The Grüneisen parameter values γ and its higher order derivatives $q\ \lambda\ and\ \xi$ calculated from the Shanker formulation [16] using Eq. (8), (10), (11) and (12). Values of $\gamma\ q\ \lambda\ and\ \xi$ get decrease with the increment in value of pressure. In the Stacey-Davis formulation they are expressed as a function of V/V_0. At extreme compression, V tends to zero, $q_\infty\ and\ \xi_\infty$ both tend to zero, but $\gamma_\infty\ and\ \lambda_\infty$ both remains positive finite.

Conclusion

The Grüneisen parameter at extreme compression, the pressure for the earth inner core and outer core boundary, the melting temperature for Fe and Co is very close. The theory of materials at (∞) infinite pressure originally due to Stacey [5,7] and further developed by Shanker et al [12,13] has been extended in the present study. Values of $\gamma\ q\ \lambda\ and\ \xi$ at finite pressures for transition metals (Fe, Co) and Calculated from the two formulations compare with each other. Results are quite similar for different transition metals (Fe, Co). Results can be produce using the input parameter given in table first. It should be emphasized that the pressure derivative of bulk modulus play the central role in determining Thermoelastic properties and equation of state of materials [1,3,21-23]. We thus obtain the following generalized expression for the higher pressure derivative of bulk modulus at infinite pressure.

Table (1) Values of input parameters for NaCl

Element	Z	γ_0	K_0	K'_0	K'_∞	γ_∞	q_0	λ_0	ξ_0
Fe(bcc)	26	1.83	187.6	5.8	3.48	1.33	1.13	6.13	4.39
Co(fcc)	27	1.77	216.5	4.7	2.82	1.24	1.21	5.91	4.20



Plots between pressure P and compression V/V_0 for Fe & Co at different temperatures

Acknowledgments

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.

References

[1] O. L. Anderson, Equation of state of solids for Geophysics and Ceramic Science, Oxford University Press, New York. 1995.

[2] M. A. Barton and F. D. Stacey, Phys. Earth Planet. Inter. 39 (1985)167.

[3] F. D. Stacey, Phys. Earth Planet Inter.89 (1995) 219.

[4] S. S. Kushwah, A. K. Upadhayay and M. P. Sharma, High Temp.-High Press.44, (2015)59.

[5] F. D. Stacey Rep. Prog. Phys. 68, (2005) 341.

[6] A. Vijay, High Temp.-High Press. 43, (2014)47

[7] Stacey F. D., Davis P. M., Phys. Earth Planet. Inter. 142, (2004) 137

[8] At'shuler L. V., Brusnikin S. E. and Kuz'menkov E. A., J. Appl. Mech. Tech. Phys. 28, (1987) 129

[9] Shanker J., Singh B. P. and Baghel H. K., Physica B 387, (2007) 409.

[10] Srivastava S. K., Sol. State Communi. 151, (2011) 1472.

[11] Kushwah S. S., Tomar Y. S. and Upadhyay A. K., J. Phys. Chem. Sol. 74, (2013) 1143.

[12] Shanker J., Dulari P. and Singh P. K., Physica B 404, (2009) 4083.

[13] Shanker J., Sunil K. and Sharma B. S., Physica B 407, (2012) 2083.

[14] Shanker J., Sunil K. and Sharma B. S., Phys. Earth Planet. Inter. 262, (2017) 41.

[15] Shanker J., Singh B. P. and Srivastava S. K., Phys. Earth Planet. Inter. 147, (2004) 333.

[16] Slater J. C., Introduction to Chemical Physics (New Yark, Mc Graw Hill,1939).

[17] Dugdale J. S. and MacDonald D. K. C., Phys. Rev. 89, (1953) 832.

[18] Vashchenka V. Ya. and Zubarev V. N., Sov. Phys. Solid State 5, (1963) 653.

[19] Barton M. A. and Stacey F. D., Phys. Earth Planet. Inter. 39, (1985) 167.

[20] Knopoff L., J. Geophys. Res. 68, (1963) 350.

[21] S. K. Sharma and B.K. Sharma Physica B405 (2010)3145.

[22] S. S. Kushwah, and N. K. Bhardwaj, Int.J. Mod. Phys. B, 24, 1187(2010).

[23] S. Kumar, S. K. Sharma, and O. P. Pandey, High Tempe- High Press. 44(2015)339.

[24] K. Sheelendra & A. Vijay, Journal of Physics and Chemistry of Solids. 123 (2018) 364-370.

[25] K. Sheelendra & A. Vijay, High Temperatures-High Pressures, Vol. 47, pp. 193–204.

[26] K. Sheelendra & A. Vijay, 9th National Conference on Thermophysical Properties (NCTP-2017) 030001-1–030001-5.