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Estimation of volume dependence of Grüneisen parameter for NaCl and ε-Fe

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The present paper proposes a new empirical expression to evaluate the values of volume dependence of the Grüneisen parameter. NaCl and ε-Fe have been taken to check the reliability of the present expression. The results obtained reveal that the present model is reliable due to a reasonably good agreement between calculated values and the values of Grüneisen parameter derived from experimental data on thermoelastic properties.

Keywords: Grüneisen parameter, Anderson-Grüneisen parameter, Thermoelastic properties

1 Introduction

The Grüneisen parameter (γ) is an important physical quantity in geophysics as it often appears in equations which describes the thermoelastic behaviour and the anharmonic properties of materials at high pressure and high temperature. The Grüneisen parameter can be considered as the measure of the change of pressure resulting from the increase of energy density at constant volume[1]. Due to lack of suitable theory and enough experimental data, it is interesting to estimate a simple method for evaluating the pressure or volume dependence of the Grüneisen parameter (γ). Many attempts[2-11] have been made to study the volume dependence of Grüneisen parameter. The Grüneisen parameter is useful to calculate the values of Debye temperature (θ_D) with the help of basic definition of Debye-Grüneisen model.

$$\gamma = -\left(\frac{d\ln\theta_D}{d\ln V}\right)_T \qquad \ldots(1)$$

and the thermal pressure can be evaluated with the following relationship:

$$P_{th} = \frac{\gamma E_{th}}{V} \qquad \ldots(2)$$

In the present study, a new empirical relationship for volume or pressure dependence of the Grüneisen parameter (γ) is proposed. The validity of present formulation to NaCl and ε-Fe is checked. The results obtained from present model with those values[12,13] of γ derived from the experimental data on thermoelastic properties are compared.

2 Theory of Grüneisen Parameter

Sharma and Sharma[14] used the following relationship for volume dependence of Anderson-Grüneisen parameter (δ_T) as:

$$\delta_T = \delta_T^{\infty} + (\delta_T^0 - \delta_T^{\infty})\left(\frac{V}{V_0}\right)^m \qquad \ldots(3)$$

where δ_T^0 and δ_T^{∞} are the values of δ_T at $P \to 0$ or $V \to V_0$ and $P \to \infty$ or $V \to 0$, respectively and m is an adjustable parameter.

Srivastava and Sinha[15] formulated the following expression for first pressure derivative of isothermal bulk modulus :

$$K_T' = K_{\infty}' + \left(K_0' - K_{\infty}'\right)\left(\frac{V}{V_0}\right)^{K_0'} \qquad \ldots(4)$$

where K'_0 and K'_{∞} are the values of first pressure derivative of isothermal bulk modulus (K_T) at atmospheric pressure i.e., $P \to 0$ and at infinite pressure i.e., $P \to \infty$ or $V \to 0$, respectively. Recently, Sharma *et al*[16]. have also used Eqs (3 and 4) to

formulate the expression to evaluate the values of volume dependence of thermal pressure for aluminium and found the good agreement with the available data for a wide range of pressures and temperatures. Thus, we have chosen these Eqs (3 and 4) in the present study to establish the relationship to predict the values of volume dependence of Grüneisen parameter.

Anderson[1] has established the following fundamental thermodynamic identity:

$$q = \delta_T - K_T' + 1 \qquad \ldots(5)$$

and q is the second Grüneisen parameter:

$$q = \left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_T \qquad \ldots(6)$$

δ_T is the Anderson-Grüneisen parameter:

$$\delta_T = -\frac{1}{\alpha K_T}\left(\frac{\partial K_T}{\partial T}\right)_P \qquad \ldots(7)$$

K_T' is the first pressure derivative of isothermal bulk modulus (K_T):

$$K_T' = \left(\frac{\partial K_T}{\partial P}\right)_T \qquad \ldots(8)$$

Eq. (5) is frequently used by many researchers[9,17-19]. Now using Eqs (3), (4) and (6) in Eq. (5), we get:

$$\left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_T = \delta_T^{\infty} + (\delta_T^0 - \delta_T)\left(\frac{V}{V_0}\right)^m - K_{\infty}' - (K_0' - K_{\infty}')\left(\frac{V}{V_0}\right)^{K_0'} + 1 \qquad \ldots(9)$$

On integration of Eq. (9), we get:

$$\frac{\gamma}{\gamma_0} = \left(\frac{V}{V_0}\right)^{\delta_T^{\infty} - K_{\infty}' + 1} \exp\left\{\left(\frac{\delta_T^0 - \delta_T^{\infty}}{m}\right)\left[\left(\frac{V}{V_0}\right)^m - 1\right] - \left(\frac{K_0' - K_{\infty}'}{K_0'}\right)\left[\left(\frac{V}{V_0}\right)^{K_0'} - 1\right]\right\} \qquad \ldots(10)$$

where all symbols are having their usual meanings.

3 Results and Discussion

Stacey[20] has listed the following basic thermodynamic identity:

$$\left(\frac{d \ln \alpha K_T}{d \ln V}\right)_T = \delta_T - K_T' \qquad \ldots(11)$$

where

$$\delta_T = \left(\frac{d \ln \alpha}{d \ln V}\right)_T \qquad \ldots(12)$$

and

$$K_T' = -\left(\frac{d \ln K_T}{d \ln V}\right)_T \qquad \ldots(13)$$

Eq. (11) has been used by various researchers[14,17,19,21-23] to discuss the nature of variation of αK_T with compression. At $P \to \infty$ or $V \to 0$, $\alpha K_T \to \infty$ only when $\delta_T - K_T'$ is negative quantity which suggests that δ_T^{∞} must be less than K_{∞}'. Thus, the value of δ_T^{∞} should be constrained according to the following relationship[24]:

$$0 < \delta_T^{\infty} < K_{\infty}' \qquad \ldots(14)$$

At $P \to \infty$ or $V \to 0$, Eq. (5) becomes:

$$q_{\infty} = \delta_T^{\infty} - K_{\infty}' + 1 \qquad \ldots(15)$$

Since $q_{\infty} \to 0$ [20,25], now Eq. (15) becomes:

$$\delta_T^{\infty} = K_{\infty}' - 1 \qquad \ldots(16)$$

Following the Stacey–Davis model[25] i.e., $K_{\infty}' = 0.6K_0'$, where K_0' is the value of isothermal bulk modulus at $P \to 0$ and room temperature i.e., $T_0 = 300$ K. The values of δ_T^{∞} obtained from Eq. (16) for both solids under consideration are enlisted in Table 1 and the calculated values satisfy the constrained [Eq. (14)].

Using Eq. (16) in Eq. (10), we get:

Table 1 — Input parameters[7,13,26-28] used in calculations

Solids	γ_0	K'_0	K'_∞	δ_T^0	δ_T^∞	M
NaCl	1.6275	5.11	3.066	5.2	2.066	2.74
ε-Fe	1.71	5.47	3.282	5.02	2.282	3

Table 2 — Values of volume dependence of Grüneisen parameter (γ) for NaCl calculated through (a) Eq. (17); and (b) values[12] of γ derived from the experimental data on thermoelastic properties

P (GPa)	V/V_0 (Ref. 12)	γ	
		(a)	(b)
0	1.0000	1.6275	1.62
1	0.9627	1.56	1.55
2	0.9324	1.50	1.51
3	0.9067	1.46	1.46
4	0.8845	1.41	1.43
5	0.8649	1.38	1.40
10	0.7910	1.25	1.27
15	0.7397	1.17	1.19
20	0.7004	1.12	1.12
25	0.6685	1.07	1.07
30	0.6416	1.04	1.03

Table 3 — Values of volume dependence of Grüneisen parameter (γ) for ε-Fe calculated through (a) Eq. (17); and (b) values[13] of γ derived from the experimental data on thermoelastic properties

P (GPa)	V/V_0 (Ref. 13)	γ	
		(a)	(b)
0.00	1.000	1.71	1.71
29.96	0.877	1.56	1.59
35.56	0.862	1.54	1.57
41.75	0.847	1.52	1.55
48.62	0.832	1.50	1.53
56.22	0.817	1.48	1.51
64.64	0.802	1.45	1.49
73.99	0.788	1.44	1.47
84.38	0.773	1.42	1.45
95.92	0.758	1.40	1.43
108.76	0.743	1.38	1.41
123.05	0.728	1.36	1.39
139.00	0.713	1.34	1.37
156.80	0.698	1.32	1.35
176.71	0.684	1.30	1.32
198.99	0.669	1.29	1.30
223.98	0.654	1.27	1.28
252.06	0.639	1.26	1.25
283.65	0.624	1.24	1.23
319.26	0.609	1.23	1.20
359.50	0.594	1.21	1.18

$$\frac{\gamma}{\gamma_0}=\exp\left\{\left(\frac{\delta_T^0-\delta_T^\infty}{m}\right)\left[\left(\frac{V}{V_0}\right)^m-1\right]-\left(\frac{K'_0-K'_\infty}{K'_0}\right)\left[\left(\frac{V}{V_0}\right)^{K'_0}-1\right]\right\} \quad \ldots(17)$$

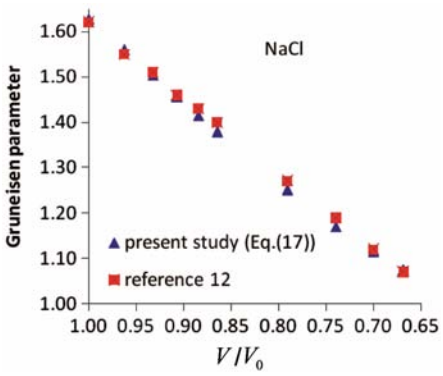

Fig. 1 — Volume dependence of Grüneisen parameter for NaCl

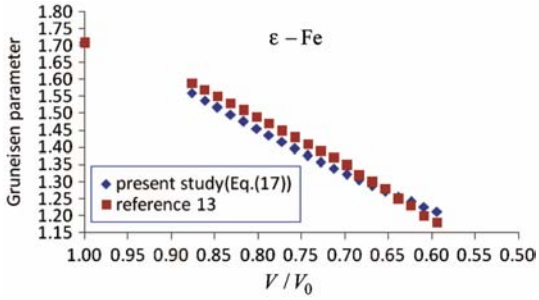

Fig. 2 — Volume dependence of Grüneisen parameter for ε-Fe

where all symbols are having their usual meanings.

The values of input parameters[7, 13, 26-28] are enlisted in Table 1. We have calculated the values of Grüneisen parameter through Eq. (17) for NaCl and ε-Fe. The results obtained through Eq. (17) are compared with the values[12,13] of γ derived from the experimental data on thermoelastic properties in Tables 2 and 3 for NaCl and ε-Fe, respectively. For direct vision we have also plotted the graphs for Grüneisen parameter versus volume along with those values of γ derived from the experimental data on thermoelastic properties in Figs 1 and 2 for NaCl and ε-Fe, respectively. Figures 1 and 2 reflect that as the volume decreases the value of Grüneisen parameter is decreased and the good agreement with those values[12,13] of γ derived from the experimental data on thermoelastic properties thus supports the validity of the present model.

4 Conclusions

In conclusion, we have thus proposed a new simple and straightforward empirical relationship to calculate the values of Grüneisen parameter γ for NaCl and ε-Fe under wide range of pressure. It is found that the results obtained through Eq. (17) are compatible with

those values[12,13] of γ derived from the experimental data on thermoelastic properties throughout the wide range of pressure for both solids under consideration. The results obtained through Eq. (17) are consistent with those values[12,13] of γ derived from the experimental data on thermoelastic properties.

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