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Analysis of Burakovsky – Preston Model For The Grüneisen Parameter of Geophysical Minerals

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Abstract

We present an analysis of the volume dependence of Grüneisen parameter and its higher order derivatives q and ƛ for five geophysical minerals viz. MgO, CaO, $MgSiO_3$, $CaSiO_3$ and Pyrope garnet ($Mg_3Al_2Si_3O_{12}$). The Burakovsky – Preston model has been used for representing gamma as a function of volume for the entire range of compressions. We have determined and reported values of γ, q and ƛ at different values of volume compressions. Values of these thermoelastic parameters (γ, q and ƛ) have been transformed to the corresponding pressures using the Holzapfel equation of state for the minerals under study.

Keywords: Grüneisen parameter ; Higher order derivatives; Equation of State ; Burakovsky – Preston model; Geophysical minerals.

1. Introduction

The Grüneisen parameter γ is an important physical quantity related to thermoelastic properties of solids [1, 2]. It also plays an important role in condensed matter physics, shock wave physics and geophysics [3, 4]. The pressure dependence of Grüneisen parameter (γ) is required to predict the thermoelastic behaviour, equation of state and melting of solids at high pressures [5-7]. The Grüneien parameter has both microscopic and macroscopic definitions. The microscopic definition relates it to the vibrational frequencies of the atom in a crystal lattice.

$$\gamma = -\frac{d\ln\omega_i}{d\ln V} \tag{1}$$

and macroscopic definition in terms of thermoelastic properties

$$\gamma = \frac{\alpha K_T V}{C_V} = \frac{\alpha K_S V}{C_P} \qquad (2)$$

In the present study we determine the Grüneisen parameter γ and its volume derivatives q and λ for some geophysical minerals viz. MgO, CaO, $MgSiO_3$, $CaSiO_3$ and $Mg_3Al_2Si_3O_{12}$ using the Burakovsky-Preston model for γ [8]. The expressions for the second order and third order Grüneisen parameters have been obtained.

2. Method of Analysis

Burakovsky and Preston [8] have developed a model for investigating the volume dependence of the Grüneisen parameter γ according to which

$$\gamma(V) = \frac{1}{2} + a_1\left(\frac{V}{V_0}\right)^{1/3} + a_2\left(\frac{V}{V_0}\right)^{n} \qquad (3)$$

Here a_1, a_2 and n are material-dependent constants with $n > 1$. Equation (3) is based on the assumption that γ is an analytic function of $V^{1/3}$ and found to accurately represent the experimentally determined low pressure behaviour of γ.

The second order and third order Grüneisen parameters q and λ are defined as follows [9, 10]

$$q = \frac{d\ln\gamma}{d\ln V} \qquad (4)$$

and

$$\lambda = \frac{d\ln q}{d\ln V} \qquad (5)$$

Expressions for q and λ are obtained using gamma from Eq. (3) in Eqs (4) and (5)

$$q = \frac{1}{\gamma}\left(\frac{1}{3}a_1\left(\frac{V}{V_0}\right)^{1/3} + a_2 n\left(\frac{V}{V_0}\right)^{n}\right) \qquad (6)$$

$$\lambda = \frac{\left(\frac{1}{9}a_1\left(\frac{V}{V_0}\right)^{1/3} + a_2 n^2\left(\frac{V}{V_0}\right)^{n}\right)}{\left(\frac{1}{3}a_1\left(\frac{V}{V_0}\right)^{1/3} + a_2 n\left(\frac{V}{V_0}\right)^{n}\right)} - q \qquad (7)$$

3. Discussion and Conclusions

Values of γ, q and λ have been calculated for five geophysical minerals viz. MgO, CaO, $MgSiO_3$, $CaSiO_3$, $Mg_3Al_2Si_3O_{12}$ with the help of equations (3), (6) and (7). The input parameters used in calculations are given in Table 1.

The pressure-volume relationships have been determined using the Holzapfel AP2 EOS [11, 12]. The Holzapfel equation of state gives the following expression for pressure-volume relationship [11, 12]

$$P = 3K_0 x^{-5}(1-x)[1+c_2 x(1-x)]\exp[c_0(1-x)] \tag{8}$$

where $x = (V/V_0)^{1/3}$, K_0 is bulk modulus at zero-pressure,

$$C_0 = -\ln\left(\frac{3K_0}{P_{FGO}}\right) \tag{9}$$

$$P_{FGO} = a_{FG}\left(\frac{Z}{V_0}\right)^{5/3} \tag{10}$$

where a_{FG} = 0.02337 GPa nm^5. The following relationship has also been obtained [11, 12]

$$C_2 = \frac{3}{2}(K_0' - 3) - C_0 \tag{11}$$

Here K_0' is the value of pressure derivative of bulk modulus at P = 0. Values of input data and EOS parameters used in computations are given in Table 2.

The results for pressure-volume relationships for five geophysical minerals are given in Table 3. Variations of the Grüneisen parameter γ and its higher order derivatives represented by q and λ are shown in Figures 1-3. Values of γ and q both decrease with the increase in volume compression. In the limit of extreme compression (V→0), γ remains positive finite, i.e. $\gamma_\infty = 1/2$, whereas q tends to zero, i.e. $q_\infty = 0$ [13, 14]. On the other hand, we note from Figure 3 that the third order Grüneisen parameter λ first appears to increase with the volume compression, and then starts to decrease rapidly at high pressures. In the limit of infinite pressure or extreme compression (V→0), the values of λ becomes $\lambda_\infty = 1/3$. This finding is consistent with detailed analysis of λ_∞ performed by Shanker et al [13, 14].

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Table 1 : Values of input parameters γ_0, a_1, a_2 and n = 1.5 for some geophysical minerals.

Mineral	γ_0	$a_1 = a_2$
MgO	1.54	0.52
CaO	1.35	0.425
$MgSiO_3$	1.5	0.50
$CaSiO_3$	1.92	0.71
$Mg_3Al_2Si_3O_{12}$	1.19	0.345

Table 2 : Values of input parameters used in computation for the Holzapfel AP2 EOS.

Mineral	V_0 (cm^3/mol)	K_0(GPa)	K'_0	P_{FG0} (GPa)	C_0	C_2
MgO	11.25	162	4.15	2626	1.69	0.04
CaO	16.75	111	4.85	2370	1.963	0.812
$MgSiO_3$	23.85	261	4.0	3449	1.483	0.017
$CaSiO_3$	27.45	232	4.8	3492	1.613	1.087
$Mg_3Al_2Si_3O_{12}$	112.6	172.8	4.0	8432	2.789	- 1.289

Table 3 : Pressure-volume relationships for some geophysical minerals determined using the Holzapfel equation of state.

V/V_0	Pressure (GPa)				
	MgO	CaO	$MgSiO_3$	$CaSiO_3$	$Mg_3Al_2Si_3O_{12}$
1.00	0	0	0	0	0
0.90	21.22	15.05	33.92	31.37	22.47
0.80	57.18	42.01	90.65	87.11	60.18
0.70	119.8	91.10	188.1	187.7	125.5
0.60	233.4	183.9	363.1	375.8	244.2
0.50	453.9	370.5	698.3	749	476.2

0.40	925.8	783.1	1407	1562	981.9
0.30	2107	1848	3115	3618	2291
0.20	6006	5467	8834	10433	6882
0.10	30179	28500	43292	52192	39042

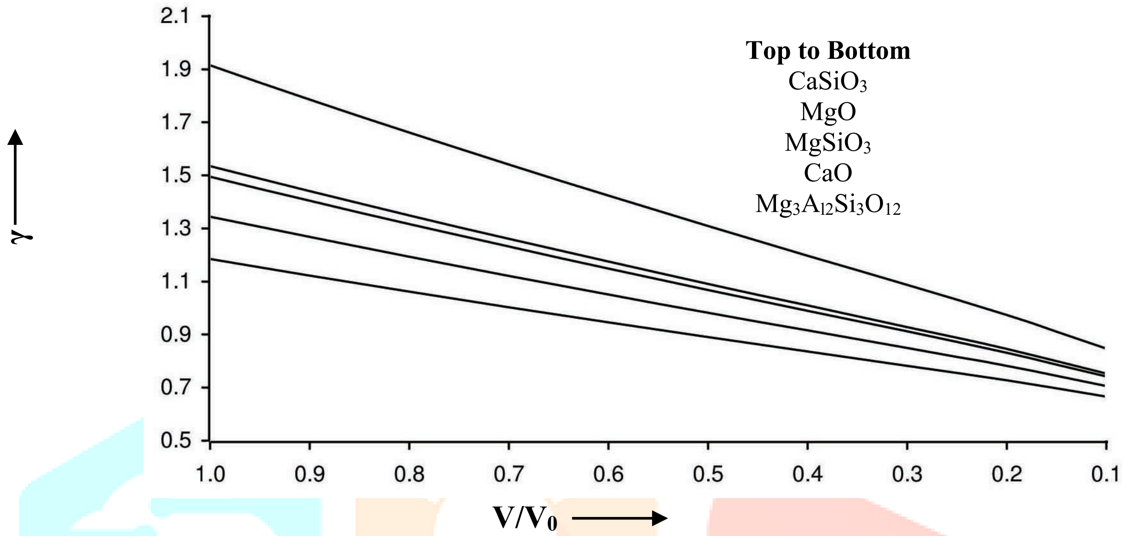

Figure 1 : Plots between the Grüneisen parameter (γ) and volume compression (V/V_0) for geophysical minerals.

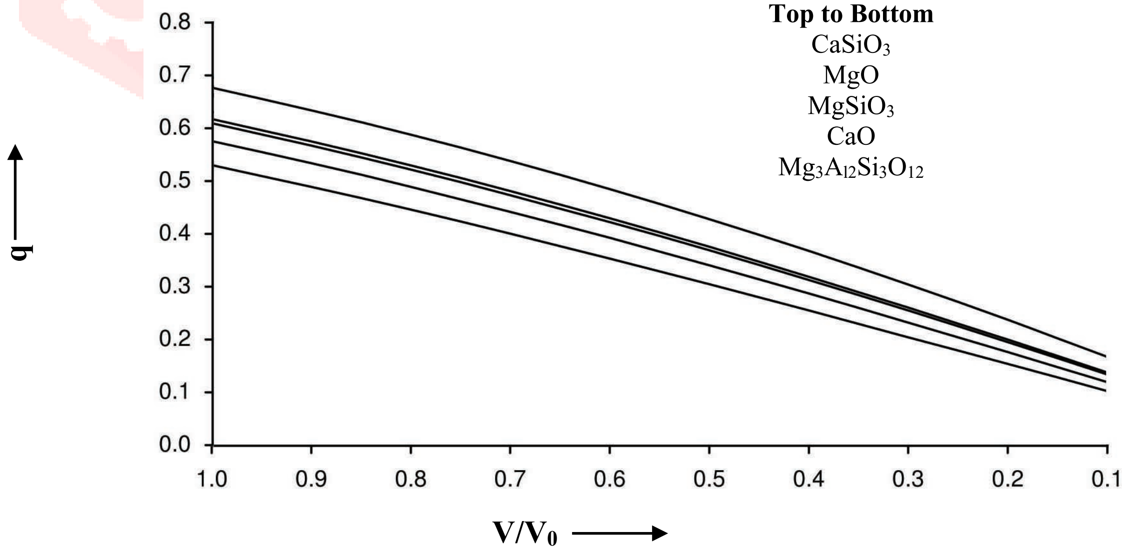

Figure 2 : Plots between second order Grüneisen parameter (q) and volume compression (V/V_0) for geophysical minerals.

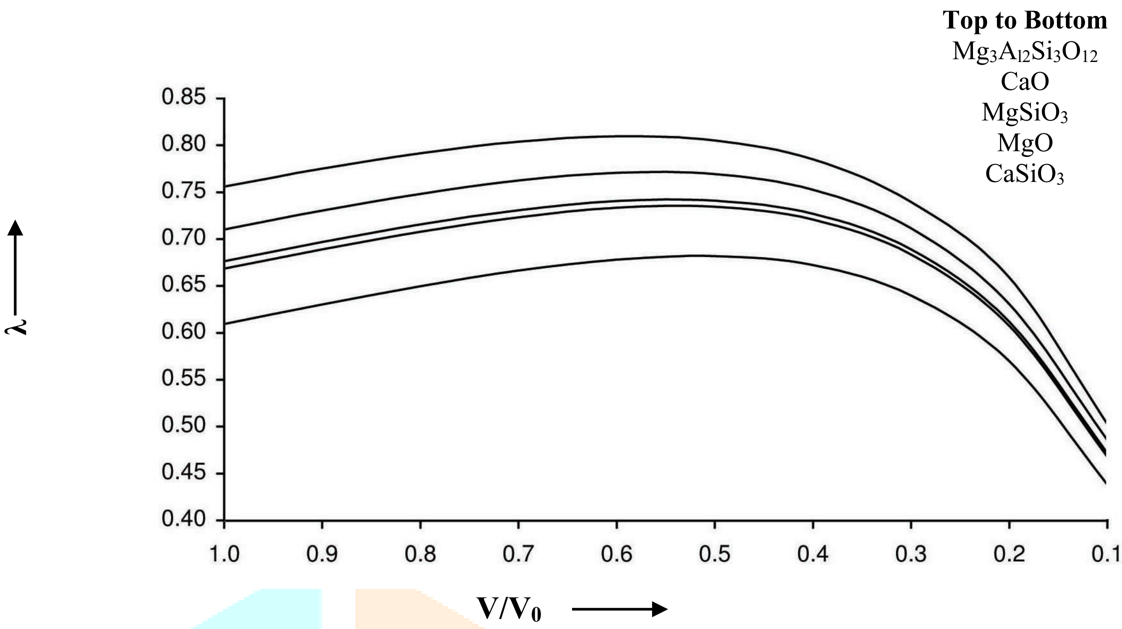

Figure 3 : Plots between the third order Grüneisen parameter (λ) versus volume compression (V/V_0) for geophysical minerals.

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