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Analysis Of Melting Temperatures Of Geophysical Minerals At High Pressures

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Abstract

We have investigated some geophysical minerals viz. CaO, $CaSiO_3$, $MgSiO_3$, $Mg_3Al_2Si_3O_{12}$ present in the lower mantle of the Earth. We have used the Holzapfel AP2 EOS for determining pressure, bulk modulus and its pressure derivative at different values of volume compression. Values of Grüneisen parameter as a function of volume are determined using the generalized free-volume formula. The Burakovsky-Preston model for the volume dependence of gamma has been used in the Lindemann law for determining melting temperatures of the geophysical minerals up to very high pressures.

Keywords : Geophysical minerals, Holzapfel AP2 EOS, Grüneisen parameter, Generalized free-volume formula, Burakovsky-Preston model, Lindemann law of melting.

1. Introduction

The Grüneisen parameter γ is an important physical quantity related to thermoelastic properties of materials (Anderson, 1995, Stacey and Davis, 2004). For determining melting temperatures of solids at high pressures, we use the Lindemann law of melting (Lindemann, 1910) which gives the following relationship

$$\frac{d\ln T_m}{d\ln V} = -2\left(\gamma - \frac{1}{3}\right) \quad (1)$$

where T_m is the melting temperature at pressure P. For integrating Eq (1) with respect to V, we need to know values of γ at different volume compressions. We use the Holzapfel AP2 EOS (Holzapfel, 1998) which holds accurately well for the entire range of pressures up to extreme compression (V→0 in the Thomas-Fermi model). The results for P, K, $K' = dK/dP$ obtained from the Holzapfel equation are used in the generalized free-volume formula (Stacey, 2005) to obtain gamma as a function of volume. The model due to Burakovsky and Preston (2004) is used to express γ as a function of volume.

The Burakovsky-Preston model is used in the Lindemann law for determining melting temperatures of geophysical minerals viz. CaO, $CaSiO_3$, $MgSiO_3$, $Mg_3Al_2Si_3O_{12}$ in the range of pressure relevant to the pressures in the lower mantle of the Earth.

2. Method of analysis

The equation of state due to Holzapfel (1998) is given below

$$P = 3K_0 x^{-5}(1-x)[1 + C_2 x(1-x)]\exp[C_0(1-x)] \quad (2)$$

where $x = (V/V_0)^{1/3}$, K_0 is the value of bulk modulus K at P = 0 and

$$C_0 = -\ln\left(\frac{3K_0}{P_{FG0}}\right) \quad (3)$$

$$P_{FGO} = a_{FG}\left(\frac{Z}{V_0}\right)^{5/3} \quad (4)$$

and

$$C_2 = \frac{3}{2}(K_0' - 3) - C_0 \quad (5)$$

Here K'_0 is the pressure derivative of bulk modulus, $K' = dK/dP$ at zero pressure, P_{FGO} is the Fermi gas pressure. The parameters K_0, K'_0, C_0 and C_2 are constants for a given material. Values of parameters used in calculations are given in Table 1.

Values of gamma are determined using the generalized free-volume formula given below (Stacey, 2005).

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

where f is the free-volume parameter. At P = 0, $\gamma = \gamma_0$,

$$\gamma_0 = \frac{K'_0}{2} - \frac{1}{6} - \frac{f}{3} \qquad (7)$$

Different formulations (Barton and Stacey, 1985, Dugdale and MacDonald, 1953, Slater, 1939, Vashchenko and Zubarav, 1963) were developed for γ by taking f equal to 0, 1, 2, and 2.35. Value of f can also be determined by matching the zero pressure value of γ for the given material. Values of pressure P, bulk modulus K and pressure derivative of bulk modulus K' are determined using the Holzapfel AP2 EOS (Holzapfel, 1998) given in Table 2.

In order to investigate the values of gamma in terms of V/V_0 we have used the formula (Burakovsky and Preston, 2004) given below

$$\gamma = \gamma^{\infty} + A_1\left(\frac{V}{V_0}\right)^{1/3} + A_2\left(\frac{V}{V_0}\right)^{m} \qquad (8)$$

where A_1, A_2 and m are constants for a given material. We can assume that $A_1 = A_2$ in Eq. (8). Then at P = 0, $V=V_0$, $\gamma = \gamma_0$ we have from Eq. (8)

$$A_1 = A_2 = \frac{1}{2}\left(\gamma_0 - \frac{1}{2}\right) \qquad (9)$$

By fitting values of gamma determined from the genealized free-volume formula, we obtain different values of m for different materials given in Table 1. Now we use the Burakovsky-Preston model, Eq. (8), in the Lindemann law of melting Eq. (1). Using Eq. (8) in Eq. (1) and then integrating we get

$$T_m = T_{mr}\left(\frac{V}{V_r}\right)^{-1/3} \exp\left[6A_1\left\{1 - \left(\frac{V}{V_r}\right)^{1/3}\right\} + \frac{2A_1}{m}\left\{1 - \left(\frac{V}{V_r}\right)^{m}\right\}\right] \qquad (10)$$

Here T_{mr} and V_r are the values of melting temperature and volume at the reference point. For CaO and $Mg_3Al_2Si_3O_{12}$, we have $Tm_r=Tm_0$ and $V_r = V_0$. Values of T_{mr} for $CaSiO_3$ and $MgSiO_3$ are taken at 16.6 GPa and 18.2 GPa, respectively, given in Table 3. These minerals are stable only at these finite pressures, and not at zero pressure. For these two minerals V_r/V_0 is found to be 0.94.

3. Discussion and Conclusions

A remarkable feature of the Burakovsky-Preston model used in the present study is that $\gamma_{\infty} = 1/2$. Eq. (1) in the limit of infinite pressure or extreme compression then becomes

$$\left(\frac{d\ln T_m}{d\ln V}\right)_{\infty} = -\frac{1}{3} \qquad (11)$$

Eq. (11) reveals that T_m varies as $V^{-1/3}$. According to the theory of the melting of one-component plasma (OCP) which represents an ionic lattice surrounded by a gas of free electrons making the system electrically neutral. One-component plasma is the limiting state of compressing a solid as pressure becomes infinitely large. According to the theory of melting of OCP, we have Eq. (11) (Burakovsky and Preston, 2004).

The results for T_m obtained in the present study for geophysical minerals at high pressures reveal that T_m increases with the increasing pressure in a non-linear manner such that the slope dT_m/dP decreases continuously with the increase in pressure. In the limit of infinite pressure we have (Shanker et al., 2020).

$$\left(\frac{dT_m}{dP}\right)_{\infty} = 0 \qquad (12)$$

Table 1 : Values of input data used in calculations of some geophysical minerals (Gupta, 2009). References for Grüneisen parameter γ (Anderson, 1995, Shim et al., 2000, Yongtao et al., 2012) and melting temperatures T_m (Shanker et al., 1999, Wang et al., 2001).

	CaO	**$CaSiO_3$**	**$MgSiO_3$**	**$Mg_3Al_2Si_3O_{12}$**
K_0(GPa)	111	232	261	178.8
K'_0	4.85	4.80	4.00	4.00
C_0	1.963	1.613	1.483	2.789
C_2	0.812	1.087	0.017	–1.289
γ_0	1.35	1.92	1.50	1.19
P_{FGO}(GPa)	2370	3492	3449	8432
f	2.73	0.940	0.999	1.93
m	1.97	2.77	1.55	0.316
T_m(K)	2853 (at zero pressure)	2932 (at 16.6 GPa)	2794 (at 18.2 GPa)	1868 (at zero pressure)

Table 2 : Values of V/V_0, P, K and K' calculated from the Holzapfel AP2 EOS. Values of γ calculated from the generalized free-volume formula are given in the last column.

V/V_0	P(GPa)	K(GPa)	K'	γ
CaO				
1	0	111	4.85	1.35
0.95	6.443	141	4.51	1.30
0.90	15.05	179	4.22	1.25
0.85	26.57	226	3.98	1.21
0.80	42.01	286	3.77	1.16
0.75	62.82	362	3.59	1.12
0.70	91.10	461	3.43	1.09
0.65	129.9	591	3.28	1.05
$CaSiO_3$				
1	0	232	4.80	1.92
0.95	13.45	294	4.45	1.80
0.90	31.37	371	4.16	1.70
0.85	55.24	467	3.91	1.61
0.80	87.11	588	3.70	1.53
0.75	129.9	742	3.52	1.46
0.70	187.7	940	3.35	1.39
0.65	266.7	1199	3.20	1.33
$MgSiO_3$				
1	0	261	4.00	1.50
0.95	14.83	319	3.79	1.44
0.90	33.92	389	3.61	1.40
0.85	58.59	476	3.45	1.35
0.80	90.65	584	3.31	1.31
0.75	132.6	720	3.18	1.27
0.70	188.1	894	3.07	1.23
0.65	262.4	1117	2.96	1.19
$Mg_3Al_2Si_3O_{12}$				
1	0	173	4.00	1.19
0.95	9.820	211	3.81	1.18
0.90	22.47	258	3.64	1.16
0.85	38.85	316	3.49	1.14
0.80	60.18	390	3.37	1.13
0.75	88.23	482	3.25	1.12
0.70	125.5	601	3.15	1.11
0.65	175.6	757	3.06	1.10

Table 3 : Calculated values of melting temperature T_m(K) and volume compression ($V/V_r = V/V_0$) of geophysical minerals under high pressures P(GPa).

CaO

$V/V_r = V/V_0$	P(GPa)	T_m(K)
1	0	2853
0.95	6.443	3158
0.90	15.05	3499
0.85	26.57	3877
0.80	42.01	4300
0.75	62.82	4778
0.70	91.10	5315
0.65	129.9	5926

$CaSiO_3$

V/V_r	V/V_0	P(GPa)	T_m(K)
1	0.940	16.6	2932
0.95	0.893	36.3	3430
0.90	0.846	57.4	4009
0.85	0.799	87.6	4665
0.80	0.752	125.5	5426
0.75	0.705	186.2	6298

$MgSiO_3$

V/V_r	V/V_0	P(GPa)	T_m(K)
1	0.940	18.2	2794
0.95	0.893	34.1	3130
0.90	0.846	59.5	3537
0.85	0.799	91.2	3988
0.80	0.752	131.8	4505
0.75	0.705	185.7	5102

$Mg_3Al_2Si_3O_{12}$

$V/V_r = V/V_0$	P(GPa)	T_m(K)
1	0	1868
0.95	9.820	2038
0.90	22.47	2241
0.85	38.85	2413
0.80	60.18	2708
0.75	88.23	3008
0.70	125.5	3348
0.65	175.6	3754

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