ANALYSIS OF MELTING OF MGO BASED ON THE LINDEMANN – GILVARRY LAW

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We have determined melting temperatures of MgO at different pressure upto 50 GPa. The Lindemann – Gilvarry law has been used by taking into account the variation of the Grüneisen parameter with increase in pressure with the help of the reciprocal gamma relationship. The results have been found to present reasonable agreement with the experimental data.

KEYWORDS : Melting curve, Grüneisen parameter, Lindemann law, MgO.

INTRODUCTION

The Lindemann – Gilvarry law of melting can be written as follows

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

where T_m is melting temperature, γ the Grüneisen parameter, V the volume. Melting occurs when the root mean squared amplitude of atomic vibrations [$<u^2>$] is a definite fraction $(\overline{e})$ of the interatomic distance r_m at melting point T_m. Thus we can write

$$< u^2 > = (\overline{e})^2 r_m^2 \quad \dots (2)$$

The assumption that $\overline{e}$ does not change with volume or pressure simplified Eq. (2) as follows [2, 3]

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

In order to determine T_m at high pressures by integrating Eq. (3), we need an analytical function for γ (V). We use an inverse function relationship for gamma [4, 5].

We determine values of T_m for MgO at high pressures. MgO is an important geophysical mineral and useful ceramic material with wide applications [6-8]. MgO has a large value of bulk modulus equal to 162 GPa and melting temperature equal to 3000K both at zero pressure. The values of T_m increase with the increase in pressure. We determine the results for T_m of MgO at high pressures upto 50 GPa.

METHOD OF ANALYSIS

First we determine pressure volume *PV* relationship using the Stacey reciprocal *K*-primed equation of state (EOS) given below [9-11]

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

Table 1. Values of volume compression V/V_0, pressure P(GPa), bulk modulus K (GPa) its pressure derivative $K' = dK/dP$ and the Grüneisen parameter γ for MgO.

V/V_0	P (GPa)	K (GPa)	K'	γ
1.000	0.00	162	4.15	1.540
0.990	1.69	169	4.08	1.526
0.979	3.53	176	4.02	1.510
0.969	5.53	184	3.95	1.494
0.957	7.72	193	3.89	1.479
0.946	10.1	202	3.83	1.464
0.934	12.7	212	3.77	1.449
0.922	15.6	223	3.72	1.434
0.909	18.8	235	3.66	1.422
0.896	22.3	247	3.61	1.408
0.882	26.1	261	3.56	1.394
0.869	30.4	276	3.51	1.381
0.854	35.1	293	3.46	1.367
0.839	40.4	311	3.41	1.356
0.824	46.3	331	3.37	1.344
0.816	50.0	342	3.34	1.335

On integrating Eq. (4) with respect to *P*, we get

$$\frac{K}{K_0} = \left(1 - K'_\infty \frac{P}{K}\right)^{-K'_0/K'_\infty} \quad \ldots (5)$$

and further integration yields

$$\ln\left(\frac{V}{V_0}\right) = \left(\frac{K'_0}{K'_\infty} - 1\right)\frac{P}{K} + \frac{K'_0}{K'^2_\infty}\ln\left(1 - K'_\infty \frac{P}{K}\right) \quad \ldots (6)$$

For determining gamma we use the relationship [12] given below

$$\frac{1}{\gamma} = \frac{1}{\gamma_0} + K'_\infty\left(\frac{1}{\gamma_\infty} - \frac{1}{\gamma_0}\right)\frac{P}{K} \quad \ldots (7)$$

For MgO we have used $K'_0 = 4.15$, $K'_\infty = 2.49$, $\gamma_0 = 1.54$ and $\gamma_\infty = 1.08$ taken from Anderson [1]. The results for *P*, *K*, *K′* and γ of MgO at different compressions up to 50 GPa are given in Table 1. The results for γ (*V*) are well represented by the following relationship [4, 5]

$$\frac{1}{\gamma} = \frac{1}{\gamma_\infty} + \left(\frac{1}{\gamma_0} - \frac{1}{\gamma_\infty}\right)\left(\frac{V}{V_0}\right)^n \quad \ldots (8)$$

Table 2. Values of T_m (K) for MgO at different pressures, (a) calculate in present study, (b) experimental values [12].

V/V_0	P (GPa)	T_m (K)	
		(a)	(b)
1.000	0	3000	3000
0.990	1.69	3072	3050
0.979	3.53	3124	3100
0.969	5.53	3238	3200
0.957	7.72	3332	3300
0.946	10.1	3424	3400
0.934	12.7	3525	3500
0.922	15.6	3631	3600
0.909	18.8	3739	3700
0.896	22.3	3857	3580
0.882	26.1	3988	3950
0.869	30.4	4115	4100
0.854	35.1	4265	4200
0.839	40.4	4417	4400
0.824	46.3	4574	4550
0.816	50.0	4670	4650

Eq. (8) holds good for MgO with n = 2.2, using Eq. (8) in Eq. (3) and then integrating we get the following expression for melting temperature [5].

$$\frac{T_m}{T_{m_0}} = \left(\frac{\gamma}{\gamma_0}\right)^{-2\gamma_\infty/n}\left(\frac{V}{V_0}\right)^{-2\gamma_\infty+\frac{2}{3}} \quad \ldots (9)$$

Results and discussions

The calculations have been performed using K_0 = 162 GPa, $K'_0 = 4.15$, $K'_\infty = 2.49$, $\gamma_0 = 1.54$ and $\gamma_\infty = 1.08$ for MgO. The results for pressure and bulk modulus calculated from the Stacey EOS using Eqs. (4) to (6) are given in Table 1. Values of γ at different pressures have been calculated using Eq. (7). For n = 2.2, Eq. (8) yields similar results as those determined from Eq. (7) given in Table 1.

A comparison of the calculated values of T_m from Eq. (9) is presented with the experimental data [12] in Table 2.

Eq. (9) is based on the Lindemann law, Eq. (3), and the inverse gamma Eq. (8), values of T_m calculated at different pressures present good agreement with the experimental data for MgO [12]. This finding reinforces the validity of the Lindemann law and the inverse gamma relationship given by Eq. (8).

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REFERENCES

1. Anderson, O.L., *Equation of State for Geophysics and Ceramic Science*, Oxford University Press Inc., New York (1995).
2. Lindemann, F.A., *Phys. Z.*, **11**, 609 (1910).
3. Gilvarry, J.J., *Phys. Rev*., **102**, 308 (1956).
4. Srivastava, S.K., Sinha, P., Verma, N., *High Temp.-High Press*., **40**, 169 (2011).
5. Vijay, A., *High Temp.-High Press*., **43**, 47 (2014).
6. Shanker, J., Kushwah, S.S., Kumar, P., *Physica*, **B 233,** 78 (1997).
7. Kushwah, S.S., Kumar, P., Shanker, J., *Phys. Chem. Sol*., **58**, 1439 (1997).
8. Kushwah, S.S., Shanker, J., *Physica*, **B 253**, 90 (1998).
9. Stacey, F.D., *Geophys. J. Int*., **143**, 621 (2000).
10. Stacey, F.D., Davis, P.M., *Phys. Earth Planet Inter*., **142**, 137 (2004).
11. Stacey, F.D., *Rep. Prog. Phys*., **68**, 341 (2005).
12. Zerr, A., Boehler, R., *Nature* (London), **371**, 506 (1994).

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