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Pressure Dependent of Melting Temperature for MgO and Hcp Iron

Dr. Sheelendra Kumar Yadav

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

ABSTRACT

The Volume dependence of the Grüneisen parameter has been used to calculate the pressure dependence of melting temperature for MgO and hcp iron using Lindemann law. The Volume dependence of the Grüneisen Parameter has been determined using gamma volume γ(V) relationship due to Al'tshuler and reciprocal gamma-volume γ(V) relationship due to Srivastava et al. The calculations are performed between pressure range 55GPa-330GPa. The values of Melting temperature are calculated at different pressures and compared with the available data reported in the literature.

KEYWORDS: Melting temperature, Grüneisen parameter, hcp Iron, Melting curve

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1. INTRODUCTION

Anderson et al. [1] have presented an analysis of the high-pressure melting temperature of hcp iron using three different approaches viz . the Lindemann -Gilvarry law [2,3] taking in to account the volume dependence of Gruneisen parameter γ the Clausius-Clapeyron equation accounting for the liquid state of melting , and the Poirier dislocation-mediated melting [4,5]. The Lindemann-Gilvarry law, most frequently used in the recent literature, is writen as follows

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

In order to determine values of melting temperature T_m at different compressions or pressures by integrating equation (1), we need to know γ as a function of volume V. there have been various attempts [1,6-7] to develop formulations for $\gamma(V)$. There have been various attempts [6–11] 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 [12, 13–16] at extreme compression in the limit of infinite pressure. In the presented study we have selected MgO which is an important ceramic material and geophysical mineral [1], and hcp iron which is the main constituent of the earth core [8, 12, 16].

2. VOLUME DEPENDENCE OF GRÜNEISEN PARAMETER

Anderson et al.[1] have investigated an empirical relationship between γ and V for hcp iron using the laboratory data. This relationship is writer as follows

$$\gamma = 1.0505\ln V - 0.2799 \qquad (2)$$

Anderson et al. [1] reported Eq. (2) as a new result based on the experimental data for hcp iron, and used it in the Gilvarry law to determine values of T_m at different pressures. It should be emphasized here that Eq. (2) is not physically acceptable.

Dorogokupets and Oganov [15] have used the Al'tshuler relationship [6] for γ(V) in order to determine the thermoelastic properties of solids at high pressures and high temperatures. According to this relationship, we can write

$$\gamma = \gamma_\infty + (\gamma_0 - \gamma_\infty)\left(\frac{V}{V_0}\right)^n \qquad (3)$$

Where n is a constant depending on the material. γ_0 and $\gamma_\infty$are the values of γ at zero pressure and in the limit of infinite pressure respectively. V_0 is the volume V at zero pressure. On differentiation Eq.(2) gives the second order Gruneisen parameter

$$q = \frac{d\ln\gamma}{d\ln} = \left(1 - \frac{\gamma_\infty}{\gamma}\right)n \qquad (4)$$

And further differentiation yields the following expression for the third order Grüneisen parameter

$$\lambda = \frac{d\ln q}{d\ln} = \frac{\gamma_\infty n}{\gamma} \quad (5)$$

Eq. (4) reveals that q_∞ tends to zero when γ tends to γ_∞. This is consistent with the thermodynamic constraint [2,3,13]. In the limit of infinite pressure, Eq. (5) gives

$$\lambda_\infty = n \quad (6)$$

And therefore

$$\lambda\gamma = \lambda_\infty\,\gamma_\infty = \text{constant} \quad (7)$$

It has been found [2,3,13-16] that λ *and* γ both decrease with the increase in pressure. However, Eq.(7) which is based on Eq. (2) is in contradiction to this finding according to Eq. (7), λ must increase with P when γ decreases. Thus it comes evident that Eq. (2) is not valid.

In order to rectify this shortcoming, attempts have been made to use the following expression for reciprocal gamma [17-11]

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

Eq. (8) on successive differentiation yields

$$q = \frac{d\ln\gamma}{d\ln V} = n\left(\frac{\gamma}{\gamma_\infty} - 1\right) \quad (9)$$

and

$$\lambda = \frac{d\ln q}{d\ln V} = \frac{n\gamma}{\gamma_\infty} \quad (10)$$

Eq. (9) is consistent with the constraints that q_∞ tends to zero when γ tends to γ_∞ Eq. (10) gives $\lambda_\infty = n$ and

$$\frac{\lambda}{\gamma} = \frac{\lambda_\infty}{\gamma_\infty} = \text{constant} \quad (11)$$

Eq.(11) is consistent with the finding that λ and γ both decrease with the increase in pressure. For determining values of the third order Grnüeisen parameter λ at limit of infinite pressures in case of the earth lower mantle and core, Stacey and Davis [2] scaled $\frac{\lambda_0}{\lambda_\infty}$ to $\frac{\gamma_0}{\gamma_\infty}$ .This is an agreement with Eq. (11). A more critical test of an expression for γ (V) can be provide using the definition of the fourth order Grüneisen parameter ξ given below [16]

$$\xi = \frac{d\ln\lambda}{d\ln} \quad (12)$$

Eq. (11) and (12) yield

$$\frac{d\ln\lambda}{d\ln V} = \frac{d\ln\gamma}{d\ln V} \quad (13)$$

According to Eq. (13) the fourth order Grüneisen parameter ξ is equal to the second order Grüneisen parameter q. This result based on Eq. (8) is not consistent with the results for ξ and q recently reported by Shanker et al. [16]. It should be emphasized that Eq. (8) is a simplified version [18, 11] of the Stacey- Davis formulation [2] for γ(V). According to the Stacey- Davis model we can write

$$\lambda = \lambda_\infty + (\lambda_0 - \lambda_\infty)\frac{q}{q_0} \quad (14)$$

On integrating Eq. (13),we get

$$q = q_0\left[1 + \frac{\lambda_0}{\lambda_\infty}\left(\frac{V_0}{V}\right)^{\lambda_\infty} - \frac{\lambda_0}{\lambda_\infty}\right]^{-1} \quad (15)$$

And further integration gives

$$\gamma = \gamma_0\left[\frac{\lambda_0}{\lambda_\infty} - \left(\frac{\lambda_0}{\lambda_\infty} - 1\right)\left(\frac{V}{V_0}\right)^{\lambda_\infty}\right]^{-\frac{q_0}{\lambda_0 - \lambda_\infty}} \quad (16)$$

It has been found [18, 11] that if we assume

$$\lambda_0 - \lambda_\infty = q_0 \quad (17)$$

Then Eq. (16) reduces to Eq. (8), and Eq. (14) becomes compatible with Eq. (9) to (11). Eq. (17) is not satisfied by the available data [2, 16]. Eq. (14) on differentiation yields

$$\xi = \left(\frac{\lambda_0 - \lambda_\infty}{q_0}\right) q \quad (18)$$

In the present study we use Eq. (14), (15), (16) and (18) to obtain γ, q, λ and ξ for MgO and hcp iron.

3. LINDEMANN LAW OF MELTING

Lindemann law is represented by Eq. (1). We prefer Eq. (8) over Eq. (14) to be used in Eq. (1) because Eq. (8) can be integrated analytically to obtain values of T_m at different compressions. It is difficult to integrate Eq. (14) using analytical methods. Eq. (1) and (8) taken together yield on integration

$$\frac{T_m}{T_{m0}} = \left(\frac{\gamma}{\gamma_0}\right)^{-\frac{2\gamma_\infty}{\lambda_\infty}}\left(\frac{V}{V_0}\right)^{-2\gamma_\infty + \frac{2}{3}} \quad (19)$$

We have used eq. (19) to determine values of $T_m(V)$. The results are then obtained for $T_m(P)$ using the pressure-volume relationship for hcp iron[9] based on the seismic data [8].

4. RESULTS AND DISCUSSIONS

For hcp iron, we take $\gamma_0 = 1.83, \gamma_\infty = 1.33,\ K_0^{'} = 5.0\,, q_0 = 1.18$ from Stacey and Davis [8]. In Eq. (13), T_{m_0}, V_0 and γ_0 correspond to the reference or the starting point. For hcp iron the starting point is at about 55GPa and $T_{m_0} = T_m(55GPa) = 2790K$ [1]. Data have been used to obtain V(P)/V(55GPa) with the help of the Stacey reciprocal K-primed EOS[8,9].

We use the Stacey K-primed equation of state, which is based on Eq.

$$\left(\frac{P}{K}\right)_\infty = \frac{1}{K_\infty^{'}} \quad (20)$$

And can be written as follows;

$$\frac{1}{K^{'}} = \frac{1}{K_0^{'}} + \left(1 - \frac{K_\infty^{'}}{K_0^{'}}\right)\frac{P}{K} \quad (21)$$

On integration , Eq. (21) gives

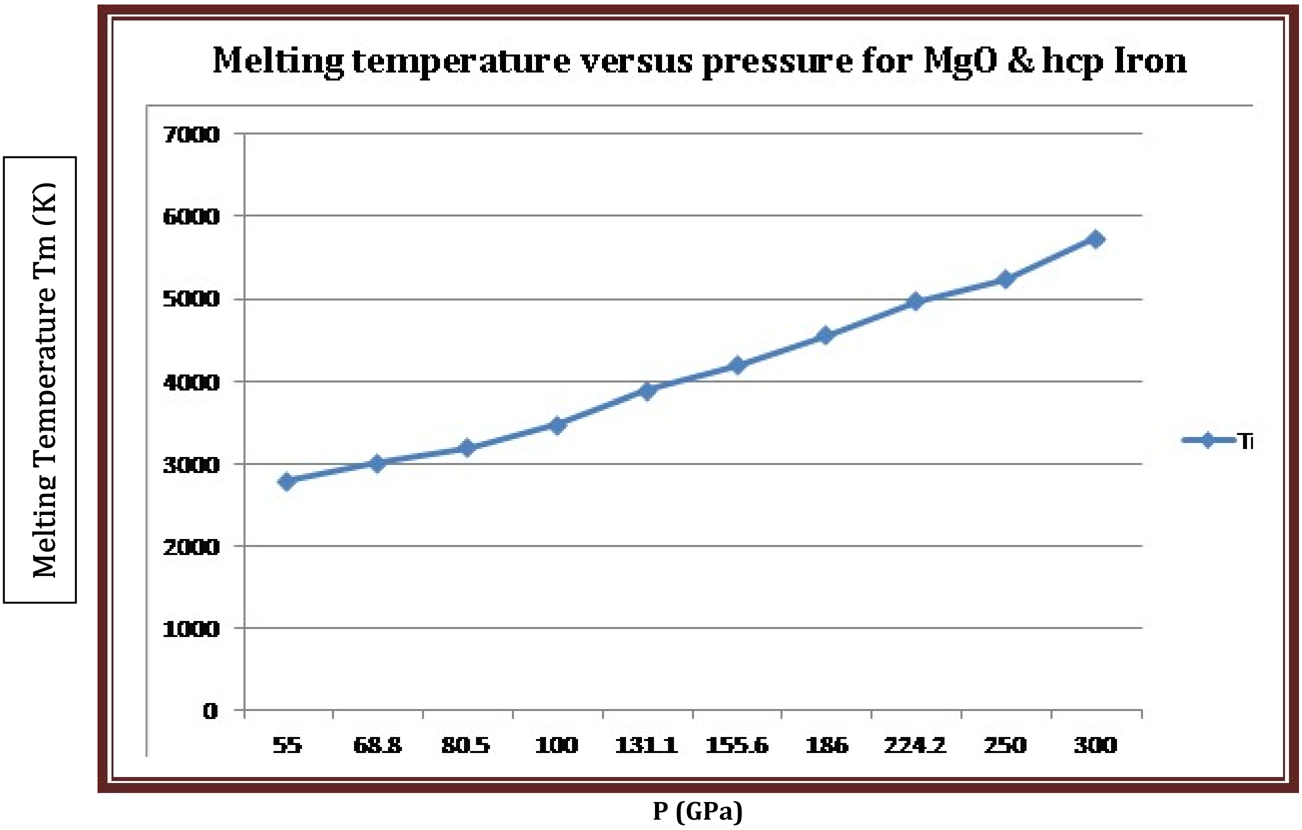
$$\frac{K}{K_0} = \left(1 - K_\infty^{'}\frac{P}{K}\right)^{-K_0^{'}/K_\infty^{'}} \quad (22)$$

Further integration of Eq. (23) gives

$$\ln\left(\frac{V}{V_0}\right) = \left(\frac{K_0^{'}}{K_\infty^{'}} - 1\right)\left(\frac{P}{K}\right) + \frac{K_0^{'}}{K_\infty^{'2}}\ln\left(1 - K_\infty^{'}\frac{P}{K}\right) \quad (23)$$

Table (1) values of volume compression V(P)/V(55GPa) at different pressures for hcp iron based on the seismic data and the Stacey equation of state [8,9], Grüneisen parameter γ calculated from Eq. (3) at n=3.66 and from Eq. (8) at n=3.14 and 2.66.

T_m	P(GPa)	V(P)/V(55GPa)	γEq.(3)	γEq.(7)
2790	55.0	1	1.571	1.557
3014	68.8	0.9686	1.544	1.532
3195	80.5	0.9452	1.526	1.515
3476	100.0	0.9117	1.502	1.493
3892	131.1	0.8679	1.473	1.467
4196	155.6	0.8394	1.457	1.452
4551	186.0	0.8092	1.441	1.438
4971	224.2	0.7774	1.426	1.424
5240	250.0	0.7587	1.418	1.417
5736	300.0	0.7275	1.405	1.406



5. CONCLUSION

The results for T_m at different pressures and compressions are given Table. Values of T_m for Mgo and hcp iron determined from Eqs. (14) and (15) are in good agreement with those obtained from the Stacey –Irvin model [8] based on the fundamental thermodynamics [1]. The most important conclusion is that the Lindemann-Gilvarry law of melting is valid for hcp iron and consistent with the thermodynamic constraints for the volume dependence of the Grüneisen parameter at extreme compression. At 330 GPa, the pressure for the Earth inner core-outer core boundary, the melting temperature for hcp iron is very close to 6000K. The importance of infinite pressure or extreme compression behavior of materials has been discussed in details by Stacey and Davis [8] pointing out the usefulness of infinite pressure constraints in determining the properties at finite pressures. Values of γ, q, λ and ξ at and hcp iron calculated from the two formulations compare with each other.

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