IOSR Journal of Applied Geology and Geophysics (IOSR-JAGG)
e-ISSN: 2321–0990, p-ISSN: 2321–0982.Volume 2, Issue 6 Ver. II (Nov-Dec. 2014), PP 52-55
www.iosrjournals.org

Volume Dependence of the Melting Temperature for Aluminium

Nidhi Verma[*1,2] S.K.Sharma[3]
1, 2 NIMS University, Shobha Nagar, Jaipur RPIIT Technical Campus, Bastara, Karnal
3 Department of Physics, Shivalik Institute of Engineering and Technology, Aliyaspur, Ambala(Haryana)

Abstract: *An attempt has been made to predict the values of melting temperature of aluminium against the volume. The melting temperatures are predicted by adding a new relationship for volume dependence of the Grüneisen ratio,* $\gamma(V)$. *The Al'tshuler's expression for* $\gamma(V)$, *extensively used in literature, is found to be inadequate for second- Grüneisen ratio and for third-Grüneisen ratio. The predicted values of melting temperature are found to present close agreement with available experimental data.*
Keywords: *Metals, Thermodynamic properties.*

I. Introduction

Sharma and Sharma [1] derived a relationship for the volume dependence of the melting temperature. The relationship is developed on the basis of the Lindemann's melting equation [2] and the Al'tshuler et al.[3] model for the volume dependence of the Grüneisen ratio. Sharma and Sharma [1] applied their relationship to estimate the volume dependence of melting temperature for aluminium up to a pressure range of 77Gpa. The aluminium (Al) has simple s-p nearly –free electronic structure and has been the subject of various theoretical and experimental investigators. Thus, the volume dependence of the melting temperature for aluminium has been both calculated [4-6] and experimentally measured [7-10] with a very secure conformity. The results obtained by Sharma and Sharma [1] present a good agreement with available experimental data [9,10]. With the increasing uses of simulations in material research and design, it is important to quantify the differences between, and accuracy of, model used in these simulations. Becker and Kramer[22] presented the results of such a comparison for four embedded atom models of aluminium that were optimized to have good liquid properties, particularly the melting temperatures. The effect of temperature and volume were systematically examined in the melts for bulk thermodyamic quantities, pair correlation function and structure factors and diffusion coefficient for each interatomic potential. These were then compared with experimental values and it was found that they were fit with similar sets of data.The present study improves the calculation made by previous workers [1]. We used a more dependable model for volume dependence of the Grüneisen ratio in place of traditionally used expression, given by Al'tshuler et.al.[3]. The method of analysis is described in section. II and results are discussed in section.III.

II. Method Of Analysis

The Al'tshuler model [3] is inadequate when we consider higher derivatives of the Grüneisen ratio. The Al'tshuler et al.[3] present following relationship for the volume dependence of the Grüneisen ratio (γ);

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

where subscripts "∞" and "0" refer to the values of the concern parameter at "infinite pressure" and "zero pressure", respectively. The parameter β is related to γ_0 and γ_∞ as follows [3];

$$\beta = \left(\frac{\gamma_0}{\gamma_0 - \gamma_\infty}\right) \qquad (2)$$

Since $\gamma_0 > \gamma_\infty$, therefore, $\beta > 1$. Expression (1) yields [11];

$$q + \lambda = \beta = \text{constant} \qquad (3)$$

$$\gamma\lambda = \text{constant} \qquad (4)$$

Here q is known as the second Grüneisen ratio, defined as follows;

$$q = \left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_T \qquad (5)$$

and the λ is termed as third Grüneisen ratio, defined as given below;

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

Since, γ, q and λ decrease as compression increases (volume decreases) [12,13], subsequently, eqs.(3) and (4) are not physically acceptable. Consequently, Al'tshuler formula [3] fails when we evaluate higher derivatives of the Grüneisen ratio. Therefore, results obtained by Sharma and Sharma [1] with the help of Al'tshuler relationship [3] need correction. In the present study we consider following expression as more reliable than eq.(4);

$$\frac{\gamma}{\lambda} = a \qquad (7)$$

where a is a constant. Relationship (7) can also be expressed as follows,

$$\gamma q = a\lambda q \qquad (8)$$

Using eqs.(5) and (6) in the left hand side and right hand side of eq.(8), we obtain

$$\gamma - \gamma_0 = a(q - q_0) \qquad (9)$$

The zero pressure and infinite pressure boundary conditions yields;

$$\gamma = \gamma_\infty + (\gamma_0 - \gamma_\infty)\frac{q}{q_0} \qquad (10)$$

Putting eq.(5) in eq.(10) and rearranging, we get

$$\int_{V_0}^{V} \frac{dV}{V} = \left(\frac{\gamma_0 - \gamma_\infty}{q_0\gamma_\infty}\right)\int_{\gamma_0}^{\gamma} \frac{d\gamma}{\gamma - \gamma_\infty} - \left(\frac{\gamma_0 - \gamma_\infty}{q_0\gamma_\infty}\right)\int_{\gamma_0}^{\gamma} \frac{d\gamma}{\gamma} \qquad (11)$$

which gives a reciprocal relationship for volume dependence of γ, as given below;

$$\frac{1}{\gamma} = \frac{1}{\gamma_\infty} + \left(\frac{1}{\gamma_0} - \frac{1}{\gamma_\infty}\right)\left(\frac{V}{V_0}\right)^{\frac{q_0\gamma_\infty}{\gamma_0 - \gamma_\infty}} \qquad (12)$$

It can be seen that relationship (12) overcomes the shortcomings in Al'tshuler et al. [3] expression. In other words, eq.(12) is more reliable than eq.(1).

The corresponding expressions for q and λ are obtained as given below;

$$\frac{q}{q_0} = \left(\frac{\gamma_\infty}{\gamma_0 - \gamma_\infty}\right)\left[\frac{\gamma_0}{\gamma_0 - (\gamma_0 - \gamma_\infty)\left(\frac{V}{V_0}\right)^c} - 1\right] \qquad (13)$$

and

$$\lambda = \frac{q_0\gamma_\infty}{(\gamma_0 - \gamma_\infty)\left[1 - \left(\frac{\gamma_0 - \gamma_\infty}{\gamma_0}\right)\left(\frac{V}{V_0}\right)^c\right]} \qquad (14)$$

where

$$c = \frac{q_0\gamma_\infty}{(\gamma_0 - \gamma_\infty)} = \lambda_\infty \qquad (15)$$

Expression (14) inter-relates γ and λ by following manner;

$$\gamma = \frac{(\gamma_0 - \gamma_\infty)}{q_0}\lambda \qquad (16)$$

Putting the values of γ, γ_0 and γ_∞ from eq.(16) in eq.(12), we get

$$\frac{1}{\lambda} = \frac{1}{\lambda_\infty} + \left(\frac{1}{\lambda_0} - \frac{1}{\lambda_\infty}\right)\left(\frac{V}{V_0}\right)^{\lambda_\infty} \qquad (17)$$

Eq.(17) is the combination of eqs.(103) and (104) of Stacey and Davis[12] , those are applied successfully to the core condition. Eq.(17) is equally applicable for isothermal and adiabatic conditions. This reflects the choice of eq.(12) in place of eq.(1) is a justifiable.

The Lindemann's melting equation is given as follows [2];

$$\left(\frac{d\ln T_m}{d\ln V}\right)_T = \frac{2}{3} - 2\gamma(V) \tag{18}$$

where T_m is the melting temperature. Eq.(18) can also be written as given below;

$$\frac{dT_m}{T_m} = \frac{2}{3} d\ln V - 2\gamma(V) d\ln V \tag{19}$$

Using eq.(12) in eq.(19) and integrating it, we get following expression for volume dependence of the melting temperature;

$$\left(\frac{T_m}{T_{m0}}\right) = \left(\frac{\gamma}{\gamma_0}\right)^{-2\gamma_\infty/m} \left\{\frac{V(T_m,P)}{V(T_{m0},0)}\right\}^{(2/3)-2\gamma_\infty} \tag{20}$$

Where T_{m0} and T_m are the melting temperatures at zero pressure and at pressure P; the $V(T_{m0},0)$ and $V(T_m,P)$ are the volumes corresponding to T_{m0} and T_m, respectively. The value of $(V(T_m,P)/V(T_{m0},0))$ can be obtained by following relationship [1];

$$\left(\frac{V(T_m,P)}{V(T_{m0},0)}\right) = \frac{V(T_m,P)}{V(T_r,P)} \times \frac{V(T_r,P)}{V(T_r,0)} \times \frac{V(T_r,0)}{V(T_{m0},0)} \tag{21}$$

Here T_r =300K, the reference temperature. Sharma and Sharma [1] used following expressions to evaluate eq.(21);

$$\alpha(T,P) = \alpha(T_r,0)\left\{\frac{V(T_r,P)}{V(T_r,0)}\right\}^{\delta_{T\infty}} \times \exp\left\{\frac{\delta(T_r,0)-\delta_{T\infty}}{k}\left[\left\{\frac{V(T_r,P)}{V(T_r,0)}\right\}^k - 1\right]\right\} \tag{22}$$

$$\frac{V(T_m,P)}{V(T_r,P)} = 1 - \frac{1}{\delta(T_r,0)+1} \times \ln\left[1-\alpha(T_r,P)\{\delta(T_r,0)+1\}(T_m - T_r)\right] \tag{23}$$

Here $\alpha(T_r,0)$ is the thermal expansivity at the reference temperature and at zero pressure, k is a dimensionless thermoelastic parameter which is of the order of unity, $k=1$. Relationship (22) is disclosed by Shanker et al. [14] with the help of the generalized Anderson-Isaak relationship of the Anderson-Grüneisen parameter (δ). Eq.(23) is originally due to Kushwah et al.[15]. Eqs.(21-23) yield the values of $(V(T_m,P)/V(T_{m0},0))$.Values of volume ratio $(V(T_r,P)/V(T_r,0))$ are extracted from literature [10]. Putting these values in eq.(20) we estimate the volume dependence of the melting temperature for aluminium.

III. Results And Discussion

Using the same input parameters as used by Sharma and Sharma [1], we estimated the values of volume dependence of the melting temperature of aluminium with the help of eq. (20). The value of the Grüneisen ratio at infinite pressure is taken to be equal to $1/2$ [13, 16-21]. This value is also used by Sharma and Sharma [1]. The value of the adjustable parameter q_0 is found to be 1.1 for aluminium. Computed values of volume dependence of melting temperature for aluminium are listed in Table.1 along with available experimental data [9,10] for the sake of comparison. An agreement between theoretically predicted values and experimental values reveals the validity of our approach. Therefore, we have modified the calculation made by Sharma and Sharma [1] with the help of a new relationship for volume dependence of the Grüneisen ratio. The modified expressions and results are more dependable than presented by previous workers.

The present work gives a theoretical formalism that describes adequately the volume dependence of the melting temperature of aluminium at high pressures. The present study is probable to be suitable for describing high pressure melting behaviour of other simple metals, having an aluminium like structure .

Table.1: Calculated values through eq.(15) along with experimental data [9,10] for the melting temperature of aluminium at different pressures

P(GPa)	$\left(\frac{V(T_r,P)}{V(T_r,0)}\right)$	$\left(\frac{V(T_m,P)}{V(T_{m0},0)}\right)$	$T_m(K)$		P(GPa)	$\left(\frac{V(T_r,P)}{V(T_r,0)}\right)$	$\left(\frac{V(T_m,P)}{V(T_{m0},0)}\right)$	$T_m(K)$	
			Eq.(15)	Exp.[10]				Eq.(15)	Exp.[9]

0.0	1.0000	1.0000	1076	1076	0.0	1.0000	1.0000	1076	1076
12.1	0.8801	0.8792	1662	1650±65	27.5	0.7921	0.7897	2282	2265±90
12.7	0.8758	0.8732	1698	1640±65	35.0	0.7612	0.7586	2547	2550±105
13.9	0.8674	0.8704	1715	1820±70	46.0	0.7240	0.7224	2895	3000±120
15.0	0.8600	0.8578	1793	1750±70	60.5	0.6851	0.6828	3332	3450±140
16.1	0.8529	0.8516	1833	1820±75	68.0	0.6681	0.6640	3563	3550±145
19.2	0.8342	0.8362	1936	2050±80	77.0	0.6500	0.6447	3818	3700±150
21.3	0.8226	0.8214	2040	2050±85					
21.3	0.8226	0.8197	2052	2000±80					
21.3	0.8226	0.8227	2031	2090±85					
28.5	0.7877	0.7846	2323	2280±90					
36.0	0.7575	0.7552	2578	2600±105					
37.0	0.7538	0.7500	2625	2570±100					
44.9	0.7274	0.7251	2867	2925±120					
44.9	0.7274	0.7232	2887	2825±115					
49.3	0.7143	0.7089	3037	2900±115					

References

[1]. S.K.Sharma, B.K.Sharma, Sol. State Commun.,150/29(2010) 1367.
[2]. F.A.Lindemann, Z.Phys. 11(1910)609.
[3]. L.V.Al'tshuler, S.E.Brusnikin, E.A.Kuz'menkov, J.Appl.Mech.Tech.Phys. 28(1987)129.
[4]. J.L.Pelissier, Physica 128A (1984)363.
[5]. J.A.Moriarty, D.A.Young,M.Ross. Phys.Rev.B 30(1984)578.
[6]. Y.Zou, L.R.Chen. Phys.Status.Solidi (b) 242/1292005)2412.
[7]. A.Jayaramn,W.Klement, R.C.Newton, G.C.Kennedy, J.Phys.Chem.Sol.,24(1963)7.
[8]. J.Less, B.H.J.Williumson, Nature 208(1965)278.
[9]. R.Boehler, M.Ross, Earth Planet.Sci.Lett. 153(1997)223.
[10]. A.Hanstrom, P.Lazor, J.Alloy. Comp., 305(2000)209.
[11]. J.Shanker, B.P.Singh and H.K.Baghel, Physica B,387(2007)409.
[12]. F.D.Stacey,P.M.Davis, Phys.Earth.Planet.Inter.142 (2004) 137.
[13]. L.Burakovsky, D.L.Preston, J.Phys.Chem.Sol.65(2004)1581.
[14]. J.Shanker, B.P.Singh, K.Jitendra,Earth and Life 2/2(2007)3.http.//www.geofinds.com
[15]. S.S.Kushwah, P.Kumar, J.Shanker, Physica B 229(1996)85.
[16]. V.P.Kopyshev,Doklady Acad.Sci.,USSR, 161(1965)1067.
[17]. W.B.Hubbard, Plnetary Interiors, Van Nostrand Co.NewYork, 1984 P.34
[18]. A.C.Holt and M.Ross,Phys.Rev.B,1(1970)2700.
[19]. M.Ross,Rep.Prog.Phys.,48(1985)1.
[20]. H.Nagara and T.Nakamur, Phys.Rev.B, 31(1985)1844.
[21]. Yu.V.Petrov,High Press.Res.,11(1994)313.
[22]. C A Becker and M J Kramer,Modelling Simul. Mater. Sci. Eng.,18,07(2010)4001