Volume Dependence of the Melting Temperature for Aluminium

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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 thermodynamic 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


\[
\gamma = \gamma_\infty + (\gamma_0 - \gamma_\infty) \left(\frac{V}{V_0}\right)^\beta
\]  

(1)

where subscripts “\(\infty\)” and “0” refer to the values of the concern parameter at “infinite pressure” and “zero pressure”, respectively. The parameter \(\beta\) is related to \(\gamma_0\) and \(\gamma_\infty\) as follows [3];

\[
\beta = \frac{\gamma_0}{\gamma_0 - \gamma_\infty}
\]  

(2)

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

\[
q + \lambda = \beta = \text{constant}
\]  

(3)

\[
q \lambda = \text{constant}
\]  

(4)

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

\[
q = \left(\frac{\partial \ln \gamma}{\partial \ln V}\right)_T
\]  

(5)

and the \(\lambda\) is termed as third Grüneisen ratio, defined as given below;
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\[ \lambda = \left( \frac{\partial \ln q}{\partial \ln V} \right)_T \]  \hspace{1cm} (6)

Since, \( \gamma, q \) and \( \lambda \) 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);

\[ \frac{\gamma}{\lambda} = a \]  \hspace{1cm} (7)

where \( a \) is a constant. Relationship (7) can also be expressed as follows, \( \gamma q = a\lambda q \)  \hspace{1cm} (8)

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

\[ \gamma - \gamma_0 = a(q - q_0) \]  \hspace{1cm} (9)

The zero pressure and infinite pressure boundary conditions yields;

\[ \gamma = \gamma_\infty + \left( \gamma_0 - \gamma_\infty \right) \frac{q}{q_0} \]  \hspace{1cm} (10)

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

\[ \int_{V_0}^{V} \frac{dV}{V} = \left( \gamma_0 - \gamma_\infty \right) \int_{\gamma_0}^{\gamma} \frac{d\gamma}{\gamma - \gamma_\infty} - \left( \gamma_0 - \gamma_\infty \right) \int_{\gamma_0}^{\gamma} \frac{d\gamma}{\gamma} \]  \hspace{1cm} (11)

which gives a reciprocal relationship for volume dependence of \( \gamma \), as given below;

\[ \frac{1}{\gamma} = \frac{1}{\gamma_\infty} + \left( \frac{1}{\gamma_0} - \frac{1}{\gamma_\infty} \right) \left( \frac{V}{V_0} \right)^{\gamma_0 - \gamma_\infty} \]  \hspace{1cm} (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 \( \lambda \) are obtained as given below;

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

and

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

where

\[ c = \frac{q_0\gamma_\infty}{\gamma_0 - \gamma_\infty} = \lambda_c \]  \hspace{1cm} (15)

Expression (14) inter-relates \( \gamma \) and \( \lambda \) by following manner;

\[ \gamma = \frac{(\gamma_0 - \gamma_\infty)}{q_0} \lambda \]  \hspace{1cm} (16)

Putting the values of \( \gamma, \gamma_0 \) and \( \gamma_\infty \) from eq.(16) in eq.(12), we get

\[ \frac{1}{\lambda} = \frac{1}{\lambda_c} + \left( \frac{1}{\lambda_0} - \frac{1}{\lambda_c} \right) \left( \frac{V}{V_0} \right)^{\lambda_c} \]  \hspace{1cm} (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];
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\[
\frac{d\ln T_m}{d\ln V} = \frac{2}{3} - 2\gamma(V)
\]  (18)

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

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

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

\[
\left( \frac{T_m}{T_{m0}} \right) = \left( \frac{\gamma}{\gamma_0} \right)^{-2\gamma_{m,in}} \left[ \frac{V(T_m, P)}{V(T_{m0}, 0)} \right]^{(2/3)-2\gamma_{m,in}}
\]  (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];

\[
\left( \frac{V(T_m, P)}{V(T_{m0}, 0)} \right) = \left( \frac{V(T_m, P)}{V(T_{m0}, 0)} \right) \times \left( \frac{V(T_{m0}, 0)}{V(T_{m0}, 0)} \right)
\]  (21)

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

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

\[
\frac{V(T_m, P)}{V(T_{m0}, 0)} = 1 - \frac{1}{\delta(T_r, 0) + 1} \times \ln[1 - \alpha(T, P)\delta(T_r, 0) + 1][T_m - T_r]
\]  (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(\( \delta \)). 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 \( (V(T_m, P)/V(T_r, 0)) \) 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.

<table>
<thead>
<tr>
<th>( P(GPa) )</th>
<th>( \frac{V(T_m, P)}{V(T_r, 0)} )</th>
<th>( \frac{V(T_m, P)}{V(T_{m0}, 0)} )</th>
<th>( T_m(K) )</th>
<th>( \frac{V(T_m, P)}{V(T_r, 0)} )</th>
<th>( \frac{V(T_m, P)}{V(T_{m0}, 0)} )</th>
<th>( T_m(K) )</th>
</tr>
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<td>[100]</td>
<td>[110]</td>
<td>[120]</td>
<td>[130]</td>
<td>[140]</td>
<td>[150]</td>
<td>[160]</td>
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<tr>
<th>Volume (mm)</th>
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<th>1.0000</th>
<th>0.0</th>
<th>1.0000</th>
<th>0.0</th>
<th>1.0000</th>
<th>0.0</th>
<th>1.0000</th>
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</thead>
<tbody>
<tr>
<td>12.1</td>
<td>0.8801</td>
<td>0.8792</td>
<td>1662</td>
<td>1650±65</td>
<td>27.5</td>
<td>0.7921</td>
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<td>12.7</td>
<td>0.8758</td>
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<td>1698</td>
<td>1640±65</td>
<td>35.0</td>
<td>0.7612</td>
<td>0.7586</td>
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<td>13.9</td>
<td>0.8674</td>
<td>0.8704</td>
<td>1715</td>
<td>1820±50</td>
<td>46.0</td>
<td>0.7240</td>
<td>0.7224</td>
<td>2895</td>
</tr>
<tr>
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<td>0.8600</td>
<td>0.8578</td>
<td>1793</td>
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<td>60.5</td>
<td>0.6851</td>
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<tr>
<td>16.1</td>
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<td>0.8516</td>
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<td>1820±75</td>
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<td>2500±140</td>
<td>2500±140</td>
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<td>0.7232</td>
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<td>3037</td>
<td>2900±115</td>
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<td>2900±115</td>
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References