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A simplified treatment to calculate the melting temperature of metals under a high pressure

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Abstract. We use a simplified treatment to calculate the melting temperature of metals under a high pressure presented by Schlosser *et al* using Lindemann's law, the Debye model and the assumption that the Grüneisen parameter divided by the volume is constant. Although the same assumptions are made in this paper, the procedure for calculating the melting temperature under a high pressure for seven metals (Al, Ag, Au, Cu, Na, K and Rb) demonstrates that the method used in this paper has the same efficiency as that of Schlosser *et al* but that our method is much simpler.

1. Introduction

It is very interesting to find a method that can be used to calculate the melting temperature of metals under a high pressure efficiently and conveniently. In 1989, on the basis of Lindemann's law, the Debye model and the assumption that the ratio γ/V of the Grüneisen parameter γ to the volume V is a constant, Schlosser *et al* [1] presented a calculation method that is rather indirect with the Tait equation, the Vinet *et al* equation and the low-pressure approximation. They fitted the experimental data on the melting temperature under a high pressure for eight metals (Al, Ag, Au, Cu, Na, K, Rb and Pt), and the calculated curves of the melting temperature versus pressure using the parameters obtained by the fitting are in good agreement with the experimental values. In this paper, we present a simplified treatment of the calculation on the basis of the same starting point as that in [1]. The procedure for calculating the melting temperature under a high pressure for seven metals (Al, Ag, Au, Cu, Na, K and Rb; Pt was not included because of the scatter in the points) demonstrates that the method used in this paper has the same efficiency as that in [1] but our method is more straightforward and much simpler.

2. The calculation of the melting temperature of metals under a high pressure

According to Lindemann's law, the relationship between the melting temperature T_m and the Debye temperature Θ_D is given by

$$T_m = C V_m^{2/3} \Theta_D^2 \tag{1}$$

where C is a constant which depends on the material, and V_m is the volume at the temperature T_m. The Grüneisen parameter γ, which is a function of volume and temperature, is given in the Debye model by

$$\gamma = -\partial(\ln \Theta_D / \partial \ln V) \tag{2}$$

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and hence

$$(\partial\Theta_D/\partial V)_T = -\gamma\Theta_D/V. \tag{2a}$$

As a good approximation, we assume that γ/V is a constant, i.e.

$$\gamma/V = \gamma_{r0}/V_{r0} = \text{constant} \tag{3}$$

where γ_{r0} and V_{r0} are the Grüneisen parameter and the volume, respectively, at zero pressure and room temperature. It should be noted that our assumption of $\gamma/V = \gamma_{r0}/V_{r0}$ differs from the assumption of Schlosser *et al* that $\gamma/V = \gamma_0/V_0$. However, it is assumption (3) that leads to our simplification of working with room-temperature values of B_0 and B_0' which are known experimentally (table 1), as will be shown in the following section.

Table 1. The values of $a(T_r)$, $B_0(T_r)$, $B_0'(T_r)$ and the zero-pressure Grüneisen parameter γ_{r0}.

Metal	$a(T_r)$ [4] ($10^{-6}K^{-1}$)	$B_0(T_r)$ (kbar)	$B_0'(T_r)$	γ_{r0} This work	γ_{r0} Experimental
Al	69.0	772 [5]	3.165 [6]	2.61	2.35 [7]
Ag	58.5	1007 [5]	6.12 [8]	2.47	2.46 [9]
Au	42.6	1732 [5]	6.29 [8]	4.40	3.09 [9]
Cu	50.1	1370 [5]	5.48 [8]	1.98	1.97 [9]
Na	207	62 [6]	3.50 [6]	1.02	1.19 [10]
K	246	32 [5]	2.99 [6]	0.96	1.11 [11]
Rb	273	26.6 [6]	3.23 [6]	1.03	1.38 [10]

Hence, the following expression is given by equations (1)–(3):

$$T_m = T_{m0}X^2\exp(2\gamma_{r0}\Delta V/V_{r0}) \tag{4}$$

where $X = (V/V_{m0})^{1/3}$, $\Delta V = V_{m0} - V$, and V_{m0} is the zero-pressure volume at the melting temperature T_{m0}.

If we write

$$\xi = (V_{m0}/V_{r0})^{1/3} \qquad X_r = (V/V_{r0})^{1/3}$$

then equation (4) can be written as

$$T_m = T_{m0}X_r^2\exp[2\gamma_{r0}(\xi^3 - X_r^3)]/\xi^2. \tag{4a}$$

For $T > \Theta_D$, the pressure $P(T, V)$ is related to the isothermal pressure $P(T_r, V)$ at the reference temperature T_r (i.e. the room temperature) by [2]

$$P(T, V) = P(T_r, V) + a(T_r)B_0(T_r)(T - T_r) \tag{5}$$

where $a(T_r)$ is the volume thermal expansion coefficient at T_r and $P = 0$, and $P(T_r, V)$ is given by the Vinet *et al* [3] equation

$$P(T_r, V) = [3B_0(T_r)(1 - X_r)/X_r^2]\exp\{\tfrac{3}{2}[B_0'(T_r) - 1](1 - X_r)\} \tag{6}$$

where $B_0(T_r)$ and $B_0'(T_r)$ are the bulk modulus and its first pressure derivative, respectively, at zero pressure and room temperature. Substituting equation (6) into equation (5) and letting $P(T_{m0}, V) = 0$, we can obtain ξ; then the Grüneisen parameter γ_{r0} can be obtained by fitting the experimental data on the melting temperature under a high pressure of the metal with equations (4*a*) and (5). The theoretical curve of T_m versus P can be plotted with equations (4*a*) and (5) using the γ_{r0}-value obtained by the fitting. With the method mentioned above, we fit and calculate the melting temperatures under a high pressure of seven of the metals used in [1] (Al, Ag, Au, Cu, Na, K and Rb; Pt is discarded because its experimental points are scattered) again. The values of the parameters $a(T_r)$, $B_0(T_r)$ and $B_0'(T_r)$, which are necessary for the fitting, are all listed in table 1. The values obtained by measuring and by fitting, respectively, the Grüneisen parameter at zero pressure and room temperature are also listed in table 1.

The calculated results again show the following: for Al, Ag and Cu, the maximum relative deviations $[(T_{mc} - T_{me})/T_{me}]_{max}$ between the melting temperature T_{mc} and its experimental value T_{m0} are less than 1%; for Na and Au, they are less than 2%; for K and Rb, they are less than 4%. For the convenience of comparison, the calculated results for Al, Na and K are plotted as broken curves and their experimental data as full circles in figures 1–3. In order to save space the calculated curves of T_m against P for the remaining four metals are not given. From the above we can see that the agreement between the theoretical curves and the experimental data is satisfactory.

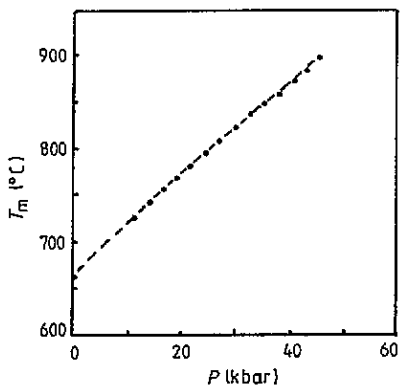

Figure 1. The curve of T_m against P for Al: ----, theory; ●, Experiment [12].

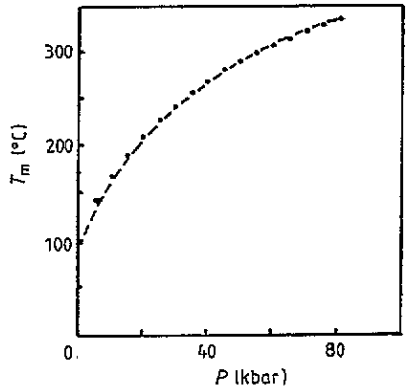

Figure 2. The curve of T_m against P for Na: ----, theory; ●, Experiment [13].

3. Conclusions

(1) The same starting point is taken both in this paper and in [1]. The differences between them are that the expression $\gamma/V = \gamma_0/V_0 =$ constant is used in [1] and $\gamma/V = \gamma_{r0}/V_{r0} =$ constant is employed in this paper. However, from the above we can see that the computational procedure used in this paper is more straightforward and simpler. In this paper, the fitted parameter γ_{r0} can be obtained directly by equations (4*a*) and (5) with the zero-pressure parameters $a(T_r)$, $B_0(T_r)$ and $B_0'(T_r)$ as well as Vinet *et al* equation. Then the calculated curves of T_m against P can be obtained. Therefore, it is unnecessary

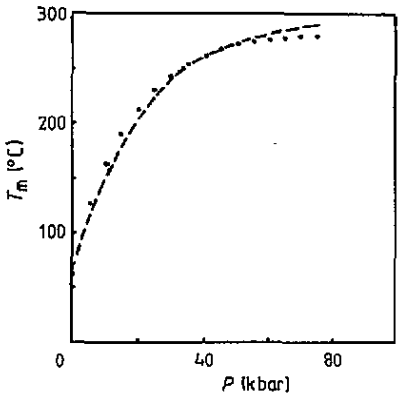

Figure 3. The curve of T_m against P for K: ----, theory; ●, Experiment [13].

to calculate tediously the values of $B_0(T_{m0})$ and $B_0'(T_{m0})$ at the melting temperature T_{m0}, as done in [1], with the Tait equation and the Vinet *et al* equation as well as the same three parameters mentioned above in order to obtain the fitted parameter γ_0. It is noteworthy that the calculated results of the melting temperature under a high pressure for the seven metals in this paper just as in [1] are satisfactory.

(2) *In this paper, the low-pressure approximation, which was made in* [1], is discarded so that the suitable pressure range is enlarged.

(3) In general, measuring the value of the Grüneisen parameter γ at room temperature is easier than that at the melting temperature. If the value of γ can be measured accurately at room temperature, then we can predict the melting temperature under a high pressure for the metal more conveniently. For example, using the experimental values of γ_{r0} listed in table 1 for Ag and Cu we can obtain predicted values that are in good agreement with the experimental data on the melting temperature.

(4) The calculations done both in [1] and in our paper indicate that the assumption that γ/V is constant is suitable for the seven metals. However, whether the assumption is generally suitable for other metals or solids needs to be tested further.

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