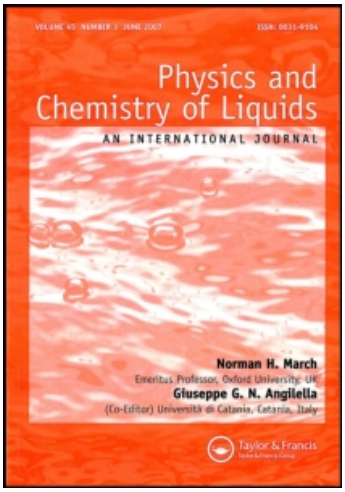

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Specific Heat of Liquid Metals

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Specific Heat of Liquid Metals

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A simple method is proposed to calculate the specific heats (C_p and C_v) of liquid metals in hard sphere reference system. The agreement between theoretical and experimental values is remarkably good for polyvalent metals.

In recent years the hard sphere model has been widely used to understand the thermodynamical properties of liquid metals. Yokoyama *et al.*[1] have made an attempt to calculate specific heat (C_p) using the Gibbs–Bogoliubov method based on a hard sphere reference system. However, their results show a serious discrepancy between theoretical and experimental values for highly polyvalent system such Sn, Pb and Bi. The authors attribute this discrepancy as due to non-alignments of structure factor of the metals from hard sphere character and also due to an explicit contribution of non-hard sphere behaviour. Recently Yokoyama, Ohkoshi and Young[2] and Ohkoshi *et al*[3] reported the calculations of specific heats C_v and C_p respectively of liquid metals using the Percus–Yevick phonon theory which in general shows an agreement between theoretical and experimental results. In the present communication, we propose a simple method based on hard sphere reference system to calculate specific heats C_p and C_v of liquid metals. In these calculations, the experimental values of coefficient of thermal expansion are used. The aim of this paper is to test the sensitivity of the present method for polyvalent liquid metals having complicated liquid structure.

The bulk entropy of liquid metals in hard sphere reference system can be expressed as

$$S = S_{\text{hs}} + S_{\text{el}}$$

with

$$S_{\text{hs}} = S_{\text{gas}} + S_{\eta} \tag{1}$$

where S_{gas} is the ideal gas entropy and S_η depends upon the packing fraction. Following Carnahan and Starling[4]

$$\frac{S_{gas}}{NK_B} = 2.5 + \mathrm{Ln}\left[\Omega\left(\frac{MKT}{2\pi\hbar^2}\right)^{3/2}\right] \tag{2}$$

and

$$\frac{S_\eta}{NK_B} = -(\xi - 1)(\xi + 3) \tag{3}$$

with

$$\xi = \frac{1}{1-\eta}$$

Thus specific heat at constant pressure $[C_p = T(dS/dT)_p]$ is described by

$$C_p = T\left(\frac{\partial S_{gas}}{\partial T}\right)_p + T\left(\frac{\partial S_\eta}{\partial T}\right)_p + T\left(\frac{\partial S_{el}}{\partial T}\right)_p \tag{4}$$

We are now able to discuss C_p by calculating all the three terms of equation (4) separately

$$\frac{1}{NK_B}\left(\frac{\partial S_{gas}}{\partial T}\right) = \frac{3}{2T} + \alpha_T$$

here α_T represents the coefficient of thermal expansion of the liquid metal and

$$\frac{1}{NK_B}\left(\frac{\partial S_\eta}{\partial T}\right) = -\frac{2(2-\eta)}{(1-\eta)^3}\frac{d\eta}{dT}$$

The value of $d\eta/dT$ can be obtained by using our empirical relations[5]

$$\eta = 0.56 - \alpha\frac{T}{T_m}$$

Thus

$$\frac{1}{NK_B}\left(\frac{\partial S_\eta}{\partial T}\right) = \frac{2(2-\eta)\alpha}{(1-\eta)^3 T_m}$$

In non-interacting electron gas model the electronic contribution to the entropy is given by

$$S_{el} = Z\gamma_0 T. \quad \text{with} \quad \gamma_0 = \left(\frac{\pi K_B}{K_F}\right)^2$$

However, the contribution due to last term is negligibly small as also reported by other workers.[2,3]

The specific heat at constant volume C_v can be calculated by using the relation

$$C_p - C_v = \alpha_T^2 \Omega T B_T$$

Specific heats are then easily calculated by using the values of coefficient of thermal expansion and packing fraction. The plane values of C_p in the Table I represent the calculation from theoretically obtained packing fraction[6] and there in parenthesis are from experimentally obtained packing fraction.[7] Turning now to a comparison between calculated and experimental values of C_p, we see that the magnitude of polyvalent metals are adequately described and are marginally better than recent theoretical values using Percus–Yevick phonon theory.[3] For Sn, Pb and Bi our results are considerably improved over the values of Yokoyama *et al.*[1] in hard-sphere-system. The values obtained by using experimentally obtained packing fraction are better than by using theoretically obtained packing fraction. This may be due to the fact that theoretical packing fractions are not exactly at their melting

TABLE I

Specific heats (in units of NK_B) of liquid metals near the melting points.

Metal	η	T	C_p Ours	C_p Ref. [1]	C_p Ref. [3]	C_p Expt. [10]	γ
Mg	0.483 0.46	923 953	3.35 (3.62)	4.3	—	3.9	1.40 (1.36)
Zn	0.489 0.46	700 723	3.21 (3.56)	4.1	2.71 ± 0.03	3.78	1.30 (1.28)
Cd	0.451 0.45	673 623	3.642 (3.643)	4.1	—	3.6	1.27 (1.37)
In	0.45	433	(3.60)	3.1	3.4 ± 0.05	3.55	(1.13)
Sn	0.43	523	(3.75)	2.6	3.04 ± 0.01	3.6	(1.08)
Pb	0.46	613	(3.53)	2.9	—	3.68	(1.23)
Bi	0.412	573	(3.87)	2.3	—	3.83	(1.12)
Cu	0.410	1356.5	3.95	—	—	3.95	—
Ga	0.43	323	(3.73)	—	2.07 ± 0.08	3.35	—
Tl	0.45	588	(3.63)	—	—	3.62	(1.22)

point. Often the experimental C_p exhibits a distinct temperature dependence.[3] The different values of coefficient of thermal expansion[8,9] show insignificant change in the value of C_p, the results are not shown here. The values of C_p and the ratio of two specific heats ($\gamma = C_p/C_v$) are recorded in the Table I.

In summary, we can now say that the present procedure accounts very well for specific heats of liquid metals.

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