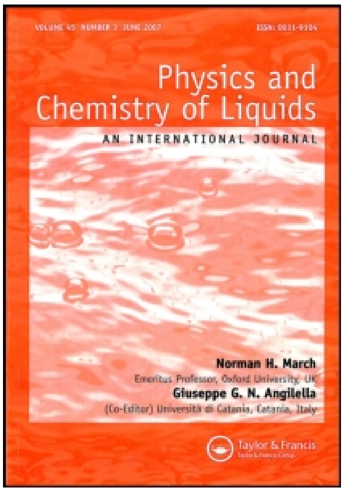

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ESTIMATION OF BULK VISCOSITY OF EXPANDED Rb

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We estimate the bulk viscosity of expanded Rb by making use of Maxwellian expression for the longitudinal viscosity. The maxwellian relaxation time for longitudinal stress correlation function is further assumed to be same as that for transverse stress correlation function. A reasonable estimate of bulk viscosity along the liquid vapour co-existence curve of Rb has been found as has been judged by comparison with experimental results of some alkali metals available at melting temperature.

Keywords: Bulk viscosity; longitudinal viscosity

1. INTRODUCTION

During the last decade there has been great interest of studying various properties of expanded metal. A great deal of experimental work [1-4] has been done to study static and dynamical properties of metals from triple point to near the critical point along the liquid-vapour co-existence curve. The main outcome of the static studies is that the numbers of nearest neighbours decrease without changing the nearest neighbour distance as one moves from triple point to critical point. Dynamically, it is found [4] that the collective density excitations observed at triple point disappears at high temperature and low density which, however, appears again for densities close to critical point.

The computer simulations for expanded Rb using pseudo-potentials with Ichumaru screening has also been done [5, 6] to study static,

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dynamical and transport properties. The results obtained for static properties are in good agreement with those obtained by experiments. The computer simulation has also provided information about density and temperature dependence of coefficient of self-diffusion and shear viscosity. Though some theoretical studies [7–8] based on similar potentials for calculation of self-diffusion and shear viscosity has been performed but till now no work has been reported for the estimate of bulk viscosity of expanded metal. Therefore, in the present work we attempt to provide some estimates of bulk viscosity by using Green Kubo relations and some known properties of expanded Rb.

2. GREEN-KUBO RELATIONS

The Green-Kubo expression relating the longitudinal stress auto correlation (LSAC) function, $S^l(t)$ to the longitudinal viscosity η_l is given by

$$\eta_l = \frac{4}{3}\eta + \eta B = \frac{1}{Vk_BT}\int_0^\infty dtS^l(t), \tag{1}$$

where

$$S^l(t) = \langle J^{xx}(t)J^{xx}(0)\rangle, \tag{2}$$

with

$$J^{xx} = \sum_{j=1}^{N}\left(\frac{p_{jx}p_{jx}}{m} + r_{jx}F_{jx}\right) - V\left(P + \frac{\partial P}{\partial \bar{E}}(E - \bar{E})\right). \tag{3}$$

In above equations p_{jx}, r_{jx} and F_{jx} are x component of velocity, position and force on jth particle, respectively. The angular brackets represent canonical ensemble average. P, V, k_B, T and m are average pressure, volume, Boltzmann constant, temperature and mass, respectively. The current chosen above is suitable for the canonical ensemble used in the present work. Expressions for $\bar{E}$ and p in terms of pair potential $U(r)$ and pair distribution function $g(r)$ are given as

$$\bar{E} = \frac{3}{2}NkT + n\int drg(r)U(r) \tag{4}$$

$$PV = k_BT - \frac{2\pi n}{3}\int_0^\infty drU'r^3g(r) \tag{5}$$

The second Green Kubo relation which relates the shear viscosity η to the transverse stress auto-correlation function $S(t)$ (TSAC) is given by

$$\eta = \frac{1}{Vk_BT}\int_0^\infty dtS(t). \tag{6}$$

where

$$S(t) = \langle J^{xy}(t)J^{xy}(0)\rangle, \tag{7a}$$

with

$$J^{xy} = \sum_{j=1}^{N}\left(\frac{p_{jx}p_{jy}}{m} + r_{jx}F_{jy}\right) \tag{7b}$$

The expression for the zeroth sum rule of LSAC function, S_0^l is obtained by putting $t = 0$ in Eq. (2). The expression thus obtained [9] is given as

$$\begin{aligned} S_0^l = {} & 4(k_BT)^2 + \frac{2\pi n}{15}k_BT\int_0^\infty drr^4g(r)(3U'' + 2U'/r) \\ & - 5(VdP/d\bar{E})(k_BT)^2 - (PV)^2 + (VdP/d\bar{E})^2(6(k_BT)^2 - \bar{E}^2) \\ & + 2PV^2(dP/d\bar{E})\left(\bar{E} - \frac{3}{2}k_BT\right), \end{aligned} \tag{8}$$

where $U' = dU(r)\backslash dr$ and $U'' = d^2U(r)\backslash dr^2$. The expression for the zeroth sum rule of the TSAC function is given as

$$S_0 = (k_BT)^2 + \frac{2\pi n}{15}k_BT\int_0^\infty drr^4g(r)(U'' + 4U'/r). \tag{9}$$

Since, the term containing $U''r^2g(r)$ in Eqs. (8) and (9) dominates at $r = \sigma$, where σ is the position of zero of the potential, one can approximately write these equations as

$$S_0^l = \frac{4}{3}(k_BT)^2 + \frac{3}{10}m\sigma^2\omega_E^2k_BT \tag{10}$$

$$S_0 = (k_BT)^2 + \frac{1}{10}m\sigma^2\omega_E^2k_BT \tag{11}$$

3. MAXWELLIAN FORM FOR LONGITUDINAL VISCOSITY

The time evolution of the stress auto correlation functions is of fundamental importance in the study of relaxation of the momentum current fluctuations and in predicting the viscosities. The exact evaluation of the time evolution of any TCF is not yet possible except for very simplified description of atomic motion. In the present work we assume Maxwellian expression for the longitudinal viscosity i.e.,

$$\eta_l = \frac{4}{3}\eta + \eta_B = \frac{n}{k_BT}S_0^l\tau \tag{12}$$

Following Barker and Gaskell [10] the maxwellian relaxation time is further assumed to be same as that for the shear viscosity and is determined by knowing the MD values of shear viscosity from the expression given as

$$\eta = \frac{n}{k_BT}S_0\tau. \tag{13}$$

S_0 and S_0^l are calculated from Eqs. (10) and (11) by using the values of ω_E^2 and σ from the work of Saroj and Tankeshwar [8] which was obtained using pseudo-potential and corresponding values of $g(r)$. The values thus obtained are given in Table I in units of ε^2, where ε is the well depth of the potential. The values of S_0 and expression (13) is used to calculate the Maxwell relaxation time τ. This maxwellian relaxation time and value of S_0^l are used to calculate the longitudinal viscosity

TABLE I Values of viscosities in centipoise

T(K)	ρ (gm/cm^3)	S_0/ε^2	S_0^e/ε^2	η_B	η	η_B/η
350.0	1.46	8.1555	23.7788	0.7659	0.4840	1.5824
373.0	1.44	8.4301	24.5192	0.6490	0.4120	1.5752
1073.0	1.13	15.0548	40.4141	0.1838	0.1360	1.3511
1373.0	0.98	15.2902	39.7298	0.1198	0.0947	1.2650
1673.0	0.83	11.7747	28.8025	0.1146	0.1030	1.1128
1873.0	0.64	6.3918	14.8989	0.0560	0.0561	0.9976

and hence the bulk viscosity. The results obtained for bulk viscosity is given in the table for six thermodynamic states along the liquid-vapour co-existence curve. It is found that bulk viscosity decreases rapidly from 0.766 to 0.056 centipoise from triple point to critical point. It is also noted that for ideal gas limit $S_0^l - (4/3)S_0$ vanishes and results in zero value of bulk viscosity.

4. COMPARISON WITH EXPERIMENT

It is interesting to note that the ratio η_B/η varies from 1.58 to about 1 as one moves from the triple point to the critical point. This ratio is significantly higher than what is known in the case of Lennard-Jones fluid. The theoretical value [11] of the ratio η_B/η using distribution function theory is simply 1.67. However, this ratio as determined by experiments [11] is around 2.4 ± 1 for liquid Na and K at the triple point density. The value of this ratio for Rb is quoted as 3.73 ± 2.24. Thus our values are not very far from the experimental values (within the experimental errors) and certainly predict the values of bulk viscosity greater than the shear viscosity. Our results seems to be of importance in future studies of bulk viscosity of expanded metals.

Acknowledgements

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