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Theoretical investigation of shear viscosity of some less simple liquid metals

Mitesh Joshi*, Manjul Kumar, P N Gajjar[1], B Y Thakore and A R Jani

Department of Physics, Sardar Patel University, Vallabh Vidyanagar-388 120, Gujarat, India
[1]Department of Physics, University of School of Sciences, Gujarat University, Ahmedabad-380 009, Gujarat, India

E-mail mjjoshi2004@yahoo.com

Abstract : Theoretical investigation of the temperature dependent Shear Viscosities are reported for some less simple liquid metals of group II-VI. Our well established model potential with recent local field correction functions of Ichimaru-Utsumi is used to derive the proper interionic pair interactions. Charged Hard Sphere reference system is employed to compute the structural data for these less simple liquid metals. Results are in good agreement when compared with the available experimental and other theoretical findings. This reveals qualitative applicability of the model potential to define atomic transport properties.

Keywords : Shear viscosity, pseudopotential, structure factor

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1. Introduction

One of the most exciting properties of a liquid is its shear viscosity. The study of viscosity of liquid metals is important for various metallurgical, industrial and biophysical applications. In the recent years considerable efforts have been done to study the shear viscosity of liquid [1–8]. In the course of theoretical investigation Molecular Dynamics (MD) also provides substantial understanding of microscopical physical mechanism underlying the dynamics of liquids [3,9]. Besides this, the distribution function as developed by Rice and Allnatt [10] is very convenient for calculation of shear viscosity due to its simple form.

The present study includes calculation of shear viscosity of liquid Mg, Zn, Ga In, Sn, and Pb metals. Since all these metals are hybridizing in a similar fashion and more or less close to *d*-shell elements, except Mg. It is interesting to focus our attention in the computation of atomic transport properties of above listed metals of group II to VI. We have used the effective pair potential based on well established model potential [11–13] which has proved its ability previously by providing excellent results of structure factor and its dependent properties.

*Corresponding Author

2. Form factor and pair potential

The essential ingredients in calculation of the shear viscosity are pair potential and pair correlation function. Proper incorporation of model potential in describing these two properties are important.

The single parametric model potential explaining the proper electron-ion interaction used in the present investigation in r-space (in Rydberg units) is given by [11],

$$W(r) = 0 \qquad r < R_C,$$
$$= \left(-\frac{2Z}{r}\right)\left[1-\exp\left(-\frac{r}{R_c}\right)\right] \quad r \geq R_C. \tag{1}$$

This model potential is the modified version of Ashcroft's empty core model potential [14].

The Effective interionic pair potential is given by

$$V(r)=\frac{Z^2}{r}\left(1-\frac{2}{\pi}\int_0^{\infty} F_N(q)\sin(qr)\,dq\right), \tag{2}$$

where $F_N(q)$, the normalized energy wave number characteristics is expressed as

$$F_N(q)=\frac{(q^2W^B(q))^2}{4\pi Zn}\left[1-\frac{1}{\varepsilon(q)}\right]\left[\frac{1}{1-G(q)}\right]. \tag{3}$$

Here, $W^B(q)$ is the Fourier transform of the corresponding bare-ion form factor in the momentum space [11] while Z, q and r_c are respectively valency, magnitude of the momentum transfer vector and the parameter of the potential. In eq. 3, $\varepsilon(q)$ denotes the dielectric function and $G(q)$ takes care for the local field correction functions. The local field correction due to Ichimaru-Utsumi (IU) [15] is used for the proper incorporation of the exchange and correlation among the conduction electrons in dielectric screening.

3. Structure factor and pair correlation function

Within a linear screening approximation, the structure factor of a liquid metal in charged hard sphere (CHS) reference system is represented as

$$S(q)=\frac{S_0(q)}{\left[1+\rho\beta\,\bar{V}(q)\,S_0(q)\right]}. \tag{4}$$

The necessary details and the expression is found in [13]. The expression for the radial distribution function based on structure factor is given by

$$g(r)=1+\left(\frac{1}{2\pi^2\rho r}\right)\int_0^{\infty} q\left\{S(q)-1\right\}\sin(qr)\,dq. \tag{5}$$

4. Shear viscosity

The shear viscosity of hard sphere liquid is be written as [16]

$$\eta_0=\eta_h+\eta_s+\eta_k. \tag{6}$$

The first term on right hand side is the contribution of the hard part of the potential expressed by

$$n_h = \frac{KT\sigma}{2g(\sigma)}\left[1+\frac{8\sigma}{5}g(\sigma)\right]D_y + \frac{96\sigma^2}{5\pi}\left[\frac{g(\sigma)KT}{\Omega}\right] \tag{7}$$

in which σ is the hard sphere diameter and D_y, Ω, ξ_s are constants defined in [16].

The contribution of soft part of the potential in shear viscosity is

$$n_s = -\frac{4\pi Mn^2}{30\xi_s}\int_0^{\infty} r^4\left(\frac{\partial^2 v}{\partial r^2}+\frac{4}{r}\frac{\partial v}{\partial r}\right) g(r)\,dr\,. \tag{8}$$

The kinetic contribution may be written as

$$n_k = |5KT|\left[1+\frac{8\sigma g(\sigma)}{5}\right] \Big/ \left[8g(\sigma)\left[\Omega+\frac{5\xi_s}{4nMg(\sigma)}\right]\right] \tag{9}$$

$g(\sigma)$ in the above expression is the specific value of pair correlation function at hard sphere diameter, hence the final expression of shear viscosity is

$$\eta = C_s(\sigma)n_0\,. \tag{10}$$

$C_s(\sigma)$ is the scaling correction term which takes into account the effect of multiple scattering.

5. Results and discussion

The constants and parameters used in the present computations for the elements of group II–VI *viz.* Mg, Zn, In, Sn, Ga, and Pb are tabulated in Table 1.

Table 1. Input parameters.

Element	Z	T (K)	Ω_0 (a.u.)^3	η_1 [16]	r_c (a.u.)
Mg	2	953	176.754	0.4525	1.2651
		1063	177.904	0.4361	1.2986
		1153	178.851	0.4237	1.3088
Zn	2	723	105.975	0.4534	1.8613
		833	107.531	0.4410	1.8704
		933	108.971	0.4300	1.8787
Ga	3	323	128.415	0.4219	1.6902
		473	130.780	0.3977	1.7005
		823	135.828	0.3466	1.7221
		1073	139.293	0.3142	1.7366
In	3	433	182.964	0.4470	1.8113
		573	185.873	0.4286	1.8208
		773	189.991	0.4036	1.8342
		973	194.590	0.3801	1.8489
Sn	4	523	191.860	0.4266	1.6921
		573	192.694	0.4212	1.6945
		973	203.301	0.3800	1.7250
		1173	203.613	0.3610	1.7259
Pb	4	613	217.771	0.4540	1.0491
		823	219.123	0.4047	1.0559
		1023	221.453	0.3699	1.0640

The resulting pair potential is shown in Figure 1. It is illustrated from Figure 1 that the depth of the pair potential is minimum for Zn and maximum for Pb while depths of rest of the elements considered here are lie in between. The distance of position of first minimum is found be higher for Pb due to higher atomic volume and valancy.

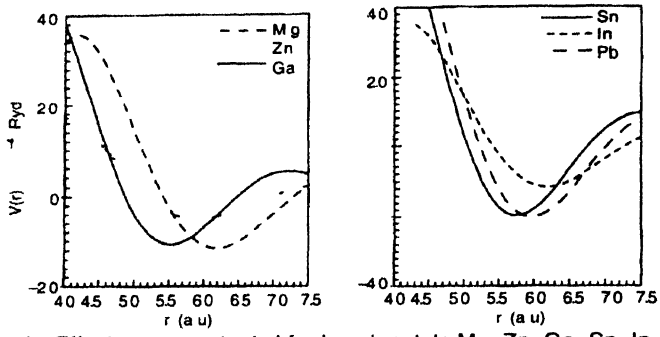

Figure 1. Effective pair potential for liquid metals Mg, Zn, Ga, Sn, In and Pb

The results obtained for the shear viscosity are narrated in Table 2 with available experimental results at temperatures near and above melting. Shear viscosity of liquid metals can also be estimated by using different formalism as done by Zahid *et al* [7] They have used the self-consistent Variational Modified Hypernetted Chain (VMHNC) integral equation based on Ornstein-Zernike equation

Table 2. Shear viscosity of liquid metals

Element	T (K)	Shear viscosity η (in cP)		
		Present	Expt [16]	Others [7]
Mg	953	1 02	1 11	1 12
	1063	0 99	–	–
	1153	0 95	–	–
Zn	723	3 34	3 85	3 64
	833	2 76	–	–
	933	2 08	–	–
Ga	323	1 66	2 14	0 98
	473	1 48	–	–
	823	1 18	–	–
	1073	0 91	–	–
In	433	1 60	1 89	1 78
	573	1 49	–	–
	773	1 38	–	–
	973	1 21	–	–
Sn	523	1 66	1 85	1 61
	573	1 64	–	–
	973	1 54	–	–
	1173	1 44	–	–
Pb	613	2.02	2 38	1 97
	823	1.94	–	–
	1023	1 85	–	–

It is immediately evident from the present study of the pair potential and pair correlation function derived from the CHS model that the computed values of shear viscosity match qualitatively well with the experimental and other theoretical findings. It is concluded here that attractive part and oscillation on the higher q values are not so significant in pair potential. In the case of shear viscosity of liquid Ga, the deviation is very large which may be due to the structural discrepancy. It is also observed that with increase in temperature the calculated shear viscosity decreases.

The estimated results are free from fitting procedures and confirm the applicability of established model potential as well as CHS method for predicting the proper structural behaviour and shear viscosity of the group II to VI elements.

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