

Theoretical Study of Structural and Dynamical Properties of Liquid Ag₇₄Ge₂₆ Alloys Using Pseudopotential Method

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The theoretical study for static structure factor and pair correlation function of liquid Ag₇₄Ge₂₆ at various temperatures computed using Ashcroft and Langreth binary structure factor method. The present calculated of pair correlation function $g(r)$ used for the study of dynamical properties such as velocity auto correlation functions (VACF) and mean square displacement (MSD) of the liquid Ag₇₄Ge₂₆ alloy will be presented based on the static harmonic well approximation. The effective interaction of the liquid is computed by our well recognized local model pseudopotential along with the local field correlation function Sarkar et al. (S). Good agreement with experimental and ab initio molecular dynamic simulation is observed for the structure factors and pair correlation functions. The obtained results of the negative dip in velocity auto correlation decrease as the various temperatures is increased and MSD concludes that the vibrating component in the atomic motion decreases as increases the temperatures. Velocity auto correlation showing the transferability of the local pseudopotential used for the liquid environment in the shell of liquid Ag₇₄Ge₂₄ binary alloys.

Keywords: Pseudopotential, Pair distribution function, Binary alloy.

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1. INTRODUCTION

Because of increasingly multiple interests of physicists, chemists, engineers, and material scientist, the study of structural and dynamical properties of liquid metals and their binary alloys are of enormous important [1-6]. The combination of noble (Au, Ag etc.) – semiconductor (Si, Ge, etc.) eutectic alloy has been widely used in fabrication of electronic and communication components. Because of high electrical and thermal conductivity of Ag₇₄Ge₂₆ alloy [1-3], Ag-Ge alloys have been considered as the potential metallic glasses and potential candidate for high power electronic device application [2, 3]. Recently, Xiong et al. [3] have successfully reported the structural and dynamical properties of liquid Ag₇₄Ge₂₆ alloy. They studied these properties at various temperatures by x-ray diffraction method and *ab-initio* MD simulations [3]. This work has encouraged us to undertake a theoretical investigation of the structural properties like structure factors ($S(q)$) and pair correlation functions $g(r)$; and dynamical properties like normalized velocity auto correlation function (VACF) and mean square displacement (MSD) of a liquid Ag₇₄Ge₂₆ binary alloy at various temperatures using model potential formalism. Here, our well recognized bare-ion model potential of the following form is used to describe electron-ion interaction [5-7],

$$V_b(q) = \frac{-4\pi Z e^2}{\Omega_0 q^2} \left[\cos(qr_c) - \frac{\exp(-1)qr_c}{(1+q^2r_c^2)} \{ \sin(qr_c) + qr_c \cos(qr_c) \} \right]. \quad (1)$$

Here Z , Ω_0 , q , e and r_c are the valence, atomic volume, wave vector, charge of an electron and parameter of the model potential, respectively. The main objective of present work is to study structural and dynamical properties

of present liquid alloy at wide range of temperatures ($T = 976$ K, 1023 K, 1073 K, and 1123 K) and judge the applicability of model potential. The exchange and correlation function due to Sarkar et al. (S) [8] is employed for inclusion of exchange and correlated effects of electrons.

2. COMPUTATIONAL METHOD

Ashcroft and Langreth have given a method for computing structure factor $S(q)$ of binary liquids [9]. They treated the system as a neutral Hard Sphere as a reference system. The equation of for computing $S(q)$ for binary system is given as [9],

$$S(q) = x \cdot S_{22}(q) + 2 \cdot [x(1-x)]^{1/2} \cdot S_{12}(q) + (1-x) \cdot S_{11}(q). \quad (2)$$

The structure factors computed by this method have been used for the computation of the pair distribution function $g(r)$. The expression used for the pair distribution function $g(r)$ is given by [9],

$$g(r) = 1 + \left(\frac{1}{2\pi^2 \rho r} \right) \int_0^\infty q [S(q) - 1] \sin(qr) dq. \quad (3)$$

For studying velocity auto correlation, a simplified equation of motion in terms of the normalized velocity autocorrelation function $\psi(t)$ as suggested by glass and Rice [10] is used

$$(d^2\psi/dt^2) + \beta_0(d\psi/dt) + \omega_0^2\psi = 0, \quad (4)$$

where

$$\psi(t) = \langle v(t)v(0) \rangle / \langle v^2 \rangle. \quad (5)$$

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Here $\langle v^2 \rangle$ is the average thermal velocity. The velocity autocorrelation satisfies specific boundary condition [5, 6, 10]. Using this condition, the solution of equation (4) is obtained as [5, 6, 10]

$$\psi(t) = \exp(-\beta_0 t/2) (\cos(\xi t) + (\beta_0/2\xi) \sin(\xi t)) \quad (6)$$

with

$$\xi^2 = \omega_0^2 - \left(\frac{\beta_0}{2}\right)^2, \quad (7)$$

$$\beta_0 = \left(\frac{MD}{k_B T}\right) \omega_0^2. \quad (8)$$

The diffusive motion of the atoms in the liquid alloy is described in terms of linear growth of the mean square distance travelled by the vibrating atoms over the time. The equation of mean square displacement $\langle r^2(t) \rangle$ is given by [5, 6],

$$\langle r^2(t) \rangle = \langle [r(t) - r(0)]^2 \rangle = 6 \langle v^2 \rangle \int_0^t \psi(t')(t' - t) dt'. \quad (9)$$

3. RESULTS AND DISCUSSION

Table 1 – Input parameters and constant for liquid $\text{Ag}_{74}\text{Ge}_{26}$ alloys at different temperature

No.	$T(\text{K})$	r_s (a.u.)	r_c (a.u.)	Ω_0 (a.u.)	$D \times 10^{-9}$ (m^2/s)
1	976	2.6059	1.356	131.94	3.222
2	1023	2.6060	1.329	131.96	3.299
3	1073	2.6088	1.331	132.39	3.382
4	1123	2.6117	1.332	132.82	3.464

The parameter of the model potential is obtained by Henine and Weaire's method [11]

$$R_c = 0.51 \left(\frac{3\Omega_0}{4\pi Z}\right)^{1/3}. \quad (10)$$

Fig. 1 shows the present results of structure factors $S(q)$ along with available ab-initio molecular dynamics and experimental data [3] and Fig. 2 shows the pair correlation functions $g(r)$ with ab-initio molecular data [3]. Here self-diffusion coefficient (D) for temperature depends has been calculated using Yokoyama method [12]. Almost the same height of the first peak is observed for structure factors and pair correlation functions for different temperatures. The computed structural properties are comparable with available results and found to be in good agreement. The present pair potential functions are used to compute the velocity auto correlation function for Ag-Ge liquid binary alloy.

The computed velocity auto correlation functions (VACF) for Ag-Ge liquid binary alloy at different temperatures are shown in Fig. 3. It is observed that when temperature is increased, the negative region of $\psi(t)$ decreases. A strong backscattering nearly between 1.45 ps to 1.43 ps and the subsequent oscillations are observed. However in the present states, backscattering is weak and oscillations converge faster. This behavior is typical of dense fluid. The VACF profile is almost same with different temperature. The correlation between the velocities is lost when the VACF reaches zero, at its large time limit. This is due to the backscattering of atoms from the

short-range and strong repulsive core collision. This system represents that the system having a lower temperature, retains its memory for a longer span of time as compared to that exhibited at the higher temperature. In the absence of experimental and other theoretical data for VACF the present results may be useful for as a reference for further investigation.

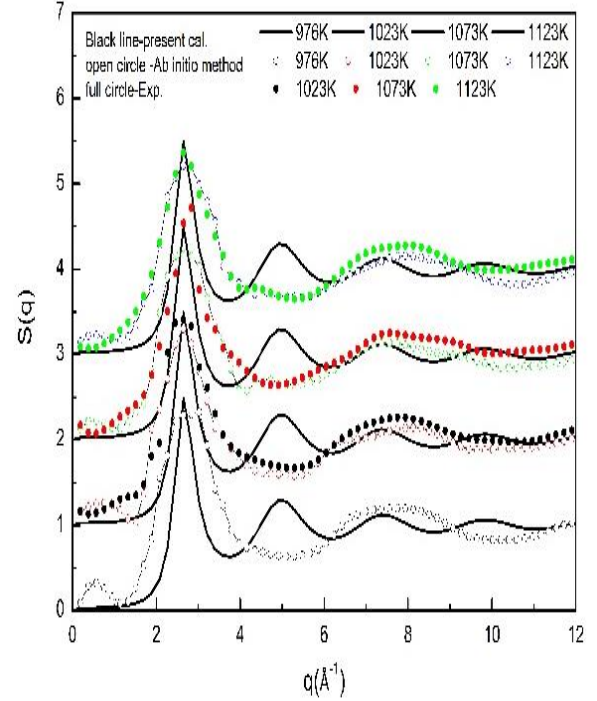


Fig. 1 – Computed structure factors $S(q)$ along with ab initio MD and experimental data [3] for $\text{Ag}_{74}\text{Ge}_{26}$ liquid alloy at different temperatures

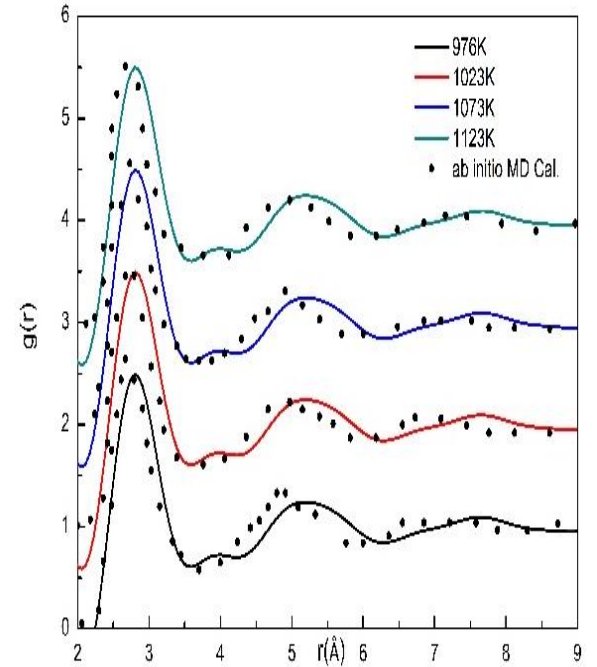


Fig. 2 – Computed pair correlation function $g(r)$ along with ab initio MD data [3] for $\text{Ag}_{74}\text{Ge}_{26}$ liquid alloy at different temperatures

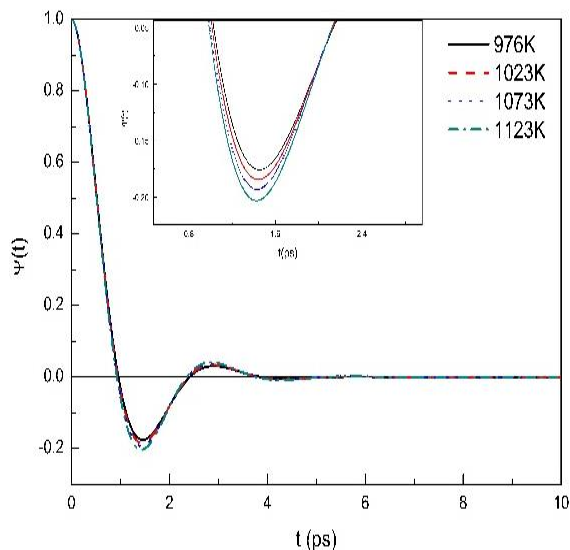


Fig. 3 – Velocity auto correlation functions (VACF) for $\text{Ag}_{74}\text{Ge}_{26}$ binary alloy at various temperatures

Fig. 4 represents computed results of mean square displacement (MSD) in the case of $\text{Ag}_{74}\text{Ge}_{26}$ liquid alloy at different temperatures. The nearly linear growth of the MSD is observed. As the temperature increases in the liquid $\text{Ag}_{74}\text{Ge}_{26}$ binary alloy the linear growth region increases, showing the sensitivity of the diffusion processes. The slope of linear growth increases with increasing temperature, gives us an idea that atom diffuses freely like gases for higher temperature.

4. CONCLUSIONS

We have reported structural and dynamical properties of the liquid $\text{Ag}_{74}\text{Ge}_{26}$ alloy. The computed total structure factor $S(q)$ and pair correlation functions $g(r)$ closely follows other such reported. The dynamical properties of present binary alloy have been also showing good trend.

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Our well identified model potential along with S local field correction functions generates consistent results regarding the structural and dynamical properties of $\text{Ag}_{74}\text{Ge}_{26}$ binary alloy. Thus, the present results confirm applicability of our model potential for study of the structural and dynamical properties of such liquid alloy.

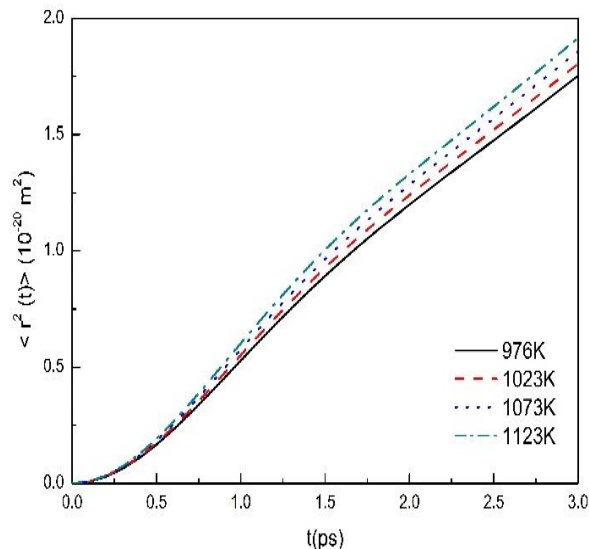


Fig. 4 – Mean square displacement (MSD) for $\text{Ag}_{74}\text{Ge}_{26}$ binary alloy at different temperatures

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