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Molecular dynamics study of $Li_{0.6}Pb_{0.4}$ binary alloy using first principle

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ABSTRACT

In this work dynamics of the liquid binary, alloy $Li_{0.6}Pb_{0.4}$ have been studied at the melting temperature by considering the system of the alloy as an assembly of effective atoms. Norm conserving pseudopotentials have been calculated using the first principle approach. Calculations performed for LiPb alloy use standard pseudopotential theory, which is second-order perturbation and include dielectric screening as well. Velocity Autocorrelation function, Phonon dispersion and power spectrum have been calculated. The calculated results are in good agreement with experimental results.

Keywords— *Liquid alloys, First-principle, Pseudopotentials, Binary*

1. INTRODUCTION

These days' liquid metal alloys are studied with collective excitations experimentally, in order to understand their dynamical behaviour. For understanding theoretical behaviour molecular dynamics using computer simulations is used [1]. Model pseudopotentials in complex formation model have been used in the past to study dynamical properties of liquid metals [2] both theoretically and experimentally. But the study of collective excitations modes in liquid alloys has received very less attention. It was the work of Jacucci and McDonald [3] carried out in $Na_{0.5}K_{0.5}$ liquid alloy which created the interest in collective excitations of liquid binary systems. Later other people also carried out the study experimentally [4, 5] and theoretical studies [6], including molecular dynamics (MD) simulations [7, 8] were also performed. In this work, a theoretical study on the structural and dynamic properties of the liquid $Li_{0.60}Pb_{0.40}$ alloy, which exhibits anomalous behaviour at complex forming stoichiometric composition.

2. THEORY

The correlation of velocities of the same particle at a time t and o is given by the velocity autocorrelation function ψ(t) which is defined as:

$$\Psi(t) = \frac{\langle v(0).v(t)\rangle}{\langle v^2\rangle} \tag{1}$$

The power spectrum of the velocity autocorrelation function is given by:

$$g(\omega) = \frac{k_B T}{mD}\int_0^t \Psi(t)\cos(\omega t)dt \tag{2}$$

One of the important thermodynamical properties of alloys is isothermal bulk modulus which is determined by calculating three elastic constants are given by:

$$\begin{aligned} C_{11} &= Q_{eff}k_B T\left(3+\frac{2I_1}{5}+\frac{I_2}{5}\right)\\ C_{12} &= Q_{eff}k_B T\left(1-\frac{2I_1}{15}+\frac{I_2}{15}\right)\\ C_{22} &= Q_{eff}k_B T\left(1+\frac{4I_1}{15}+\frac{I_2}{15}\right) \end{aligned} \tag{3}$$

Where Q_{eff} is the effective number density of the alloy and integrals I_1 and I_2 are given by:

$$I_1 = \frac{Q_{eff}}{2K_B T}\int g(r) r V'_{eff}(r) dr \tag{4}$$

$$I_2 = \frac{Q_{eff}}{2K_B T}\int g(r) r^2 V''_{eff}(r) dr \tag{5}$$

Here V'_{eff} and V''_{eff} are first and second derivatives of effective pair potential V_{eff} of the alloy and g(r) is the pair correlation function. Further isothermal bulk modulus is calculated by:

$$B_T = \frac{C_{11} + 2C_{12}}{3} \tag{6}$$

3. RESULTS

Velocity autocorrelation function has been calculated using Equation1 and the results plotted are shown in Figure1. Oscillatory behaviour of the wave function and at the same time, a negative minimum followed by decay of oscillatory behaviour is observed which is due to the scattering of atoms which are present due to short range core oscillations. After this graph becomes positive which is the result of the redevelopment of memory? Power spectrum and mean square displacement have been calculated using equation 2 and equation 3 respectively. Calculated values are plotted in figure 2 and figure 3 respectively Three elastic constants have been calculated using Equations 4 and have been further used to calculate isothermal bulk modulus using equation 7, and are shown in table 1. Phonon dispersion has been calculated using the SIESTA Code and plotted in figure 3. Showing collective excitations.

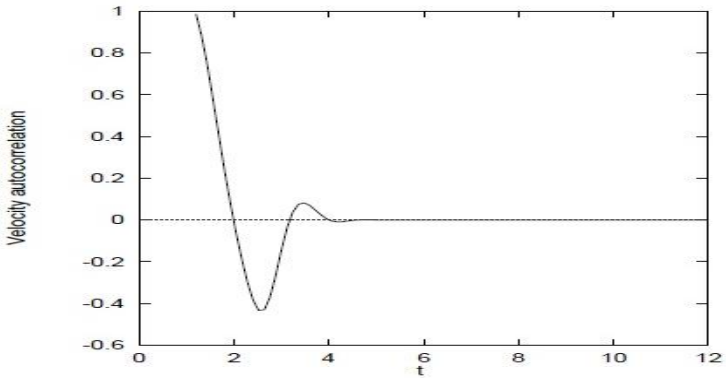

Fig. 1: Velocity autocorrelation function

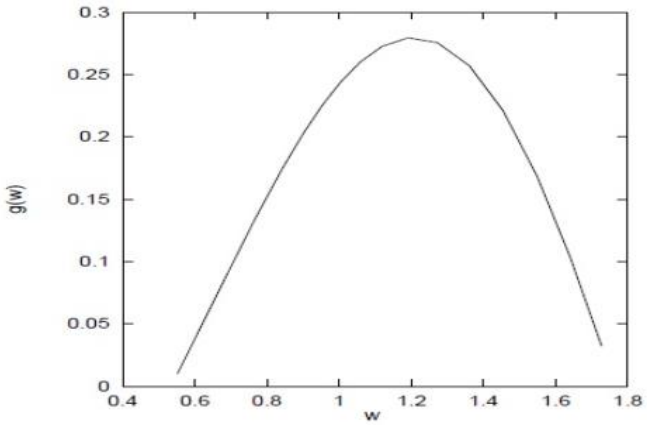

Fig. 2: Power spectrum

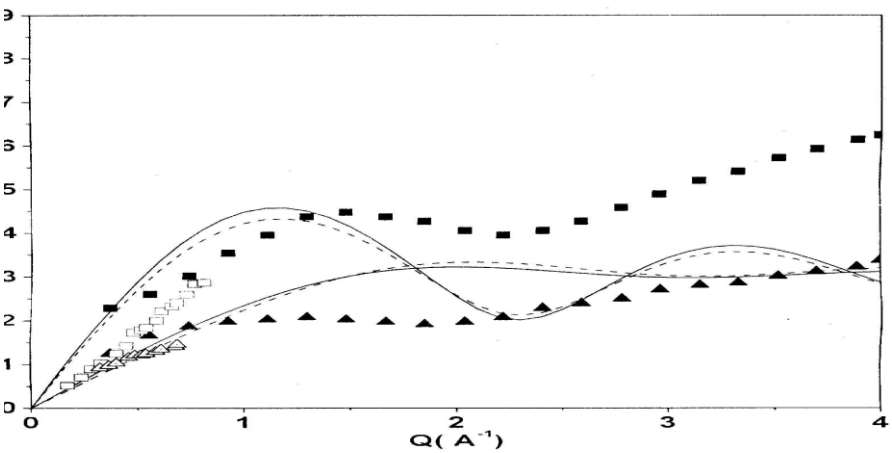

Fig. 3: Phonon Spectrum

Calculated isothermal bulk modulus is -01675 GPa/K. Calculated elastic constants are shown in table 1.

Table 1: Elastic constants

Elastic Constants	GPa
C11	49.3
C12	20.4
C22	11.3

4. CONCLUSION

Computed results in the present work are in agreement with reported MD simulations [4,8]. However, therein deviation in a longitudinal branch of the dispersion curve obtained from MD simulation which may be attributed to the difference of temperature in two cases. It is observed that the phonon dispersion obtained in the present work for liquid alloy shows well-defined collective modes similar to those found in other binary liquid alloys.

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