Structural and Collective Dynamics of Bi$_{50}$Zn$_{50}$ of binary metallic glass

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Abstract: In the present paper, structural properties, collective dynamics and elastic properties have been studied of Bi$_{50}$Zn$_{50}$ liquid metallic glass at a wide range of temperatures. Ashcroft and Langreth binary structure factor have been used to study for static structure factor and pair correlation function for present alloy. The collective excitation has been studied for longitudinal and transverses phonon modes based on our well-established model potential along with Hubbard and Beeby (HB) approach. These frequencies are expressed in terms of many-body correlation functions of atoms as well as of interatomic potential. The important ingredients in the present study are the pair-potential and pair-correlation functions. The local field correlation functions due to Hartree (H) and Farid et al (F) are employed to investigate the influence of the screening effects on the vibrational dynamics of Bi$_{50}$Zn$_{50}$ liquid metallic glass. The results for bulk modulus ($B_T$), modulus of rigidity ($G$), Poisson’s ratio ($\zeta$), Young’s modulus ($Y$), Debye temperature ($\Theta_D$), the propagation velocity of elastic waves and dispersion curves are reported. Good agreement with the experiment is observed for the structure factors and elastic properties results are consistent and confirm the applicability of model potential and self-consistent phonon theory for such studies.

1. Introduction

Binary metallic glasses show the wide range of application in the filed of engineering and material science during the several decades. They made up of components of simple metals provide us with physically interesting systems for theoretical investigations[1-4]. The simple structure of binary alloys lets us to use the pseudopotential theory to calculate the interatomic potentials among simple metal components to a high degree of precision[2-4]. Based on the knowledge of interatomic interactions we can know the mechanical, optical thermodynamic and electronic transport properties of Bi-Zn materials. The research on binary metallic glasses put on more momentum in the early ninety eighties when the continuous casting process for commercial production of metallic glasses sheets, lines and ribbons was developed [5]. The present Bi- based liquid alloy is consisting of polyanvalent metal and it's still inspiring to academician and researchers on temperature variation of physical properties such as viscosity, structural behavior, thermodynamics, mechanical, sound velocity and so many [1-6]. Bi-Zn binary alloy has occupied an important position due to their technological important and industrial application.

H Ueno et al [6] was successfully reported the structure factors and pair correlation functions of binary metallic glass Bi$_{50}$Zn$_{50}$ using x-ray diffraction, neutron and Moteno Carlo method at four different temperature [6]. This has motivated us to undertake a first-time theoretical investigation of the structural properties, phonon modes and its elastic properties of a liquid Bi$_{50}$Zn$_{50}$ binary alloy at various temperatures [6]. To incorporate the electron ion interaction we have used well recognized
model potential [7, 8]. In momentum space (q-space) the unscreened bare-ion form factor is given by [7, 8]. The model potential used to describe electron-ion interaction is form in q-space [7,8]

\[ V_b(q) = -\frac{4\pi Ze^2}{\Omega_0 q^2} \left[ \cos(qr_c) - \frac{\exp(-|q\cdot r_c|)}{1 + q^2 r_c^2} \right] \]  

(1)

Here Z, \( \Omega \), q, e and \( r_c \) are the valency, atomic volume, wave vector, charge of an electron and the parameter of the potential respectively. In the present paper, the parameter of the potential for binary alloys has been determined following the procedure \( q=\bar{q}_{\text{m}} \) method. Two local field correction functions viz. Hartree (H) [9] and Farid et al (F) [10] are used to study the screening influence on longitudinal and transverse sound velocity, isothermal bulk modulus, modulus of rigidity, Poisson’s ratio, Young’s modulus and Debye temperature at wide range of temperature (793K, 873K, 1023K 1123K) [6].

2. Theory

One of the earliest attempts to compute binary structure factor \( S(q) \) of binary metals are the system of neutral Hard Sphere as a reference system[11]. Among these the straight forward and most extensively used model is obtained from the exact solution of the Percus-Yevick (PY) equation for Hard-Sphere diameter \( \sigma \), which is obtained, to get best fit of \( S(q) \) with experimental data also known as Ashcroft-Langreth model [11]. The total structure factor \( S(q) \) of a binary mixture in terms of partial structure factors \( S_{11}(q), S_{22}(q) \) and \( S_{12}(q) \) is written by Ashcroft et al [11] and the final expression for the structure factor is written as under.

\[ S(q) = xS_{22}(y) + 2\{x(1-x)\}^{\frac{1}{2}}S_{12}(y) + (1-x)S_{11}(y) \]  

(2)

These structure factors have been used for the computation of the pair distribution function \( g(r) \). The expression for the pair distribution function \( g(r) \) is written as,

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

(3)

The fundamental ingredient, which goes into the calculation of the phonon dynamics of binary metallic glass, is the effective pair potential, which consists of two contributions. One is the direct interaction between ion given by \( \frac{Ze^2}{r} \). Other contribution is due to the indirect interaction between ions through the electron cloud and this interaction is computed using the normalized energy wave number characteristics.

In the present study the effective core radius \( r_c \) is calculated using the expression

\[ r_c^{\text{eff}} = \frac{0.51 r_{\text{eff}}}{Z_{\text{eff}}^\frac{1}{3}} \]  

(4)

and \( r_{\text{eff}} \) is given by

\[ r_{\text{eff}} = (x \cdot r_A^3 + (1-x) \cdot r_B^3)^{\frac{1}{3}} \]  

(5)

where \( r_A \) and \( r_B \) are the Wigner-seitz radii of A and B atoms respectively.

The effective ion-ion interaction is given as,

\[ V(r) = \frac{Z^2 e^2}{r} + \frac{2}{\pi} \int dq F(q) \exp(iq \cdot r), \]  

(6)
where $F(q)$ is the energy wave number characteristic. The first term gives the coulomb interaction between ions and the second term is due to the indirect interaction through the conduction electrons. This indirect interaction can be calculated using the energy wave number characteristics $F(q)$. The effective pair potential for the binary system will be obtained if the pair potentials for the single components are known. It is given by the expression

$$V_{\text{eff}}(r) = C_A^2 V_{AA}(r) + 2C_A C_B V_{AB}(r) + C_B^2 V_{BB}(r)$$

Where $V_{AA}(r)$ is the pair potential for the A-A component, $V_{BB}(r)$ is that for the B-B component and $V_{AB}(r)$ is that for the A-B component in the binary system. $C_A$ and $C_B$ are the concentration of the A and B type components respectively,

$$C_A = \frac{(1-x)\Omega_A}{(1-x)\Omega_A + x\Omega_B}$$

$$C_B = \frac{(1-x)\Omega_B}{(1-x)\Omega_A + x\Omega_B}$$

Where $\Omega_A$ and $\Omega_B$ are the molar volumes of A and B components, respectively. Another way of finding the pair potential for the binary alloy is to consider the System $x_A B_{1-x}$ is considered as a system of the effective atoms. In the present Study we have considered the effective atoms approach for computing the dispersion curves.

Two different model potentials mentioned in earlier chapters are used for the present study also. The usual form of the effective pair potential in the liquid metals and their alloys is

$$V_{\text{eff}}(r) = \frac{(Z_{\text{eff}} e)^2}{r} + \frac{\Omega_{0\text{eff}}}{\pi^2} \int dq \cdot F_{\text{eff}}(q) \cdot q^2 \left[ \sin(qr) \right]$$

Where $Z_{\text{eff}}$ is the effective valence, $\Omega_{0\text{eff}}$ is the atomic volume of the liquid metals and binary alloys, respectively. The energy wave number characteristics in expression is given by,

$$F(q) = -\frac{\Omega_{0\text{eff}} q^2}{16\pi} \left[ V_{\text{eff}}^B(q) \right]^2 \times \left[ \varepsilon_H^{\text{eff}}(q) - 1 \right] \left[ 1 + (\varepsilon_H^{\text{eff}}(q) - 1)(1 - f_{\text{eff}}(q)) \right]$$

Here $V_{\text{eff}}^B(q)$ is the effective bare ion potential, $\varepsilon_H^{\text{eff}}(q)$ the Hartree dielectric response function and $f_{\text{eff}}(q)$ the local field correction function.

In the present investigation of computing the phonon dispersion relation of alkaline earth metals, transition metals and their binary alloys, the most frequently used approach of Hubbard and Beeby [12] is taken up. With the physical argument that the product of the static pair correlation function “$g(r)$” and the second derivative of the interatomic potential “$V_{\text{eff}}(r)$” is peaked near the heard sphere diameter ‘$\sigma$’, Hubbard and Beeby have derived the expression longitudinal phonon frequencies $\omega_L(q)$ and transverse phonon frequencies $\omega_T(q)$ as [7,8,12]
Here, $\omega_E$ represents the maximum phonon frequency and is given as

$$\omega_E = \frac{4\pi n}{3M} \int_0^\infty g(r) r^2 V''_{\text{eff}} (r) dr$$

With

$$V''_{\text{eff}} (r) = \frac{4Z^2}{r^3} + \frac{\Omega_0}{\pi^2} \int_0^\infty F(q) q^3 \left[ \frac{2\sin(qr)}{qr^3} - \frac{2\cos(qr)}{r^2} - \frac{q\sin(qr)}{r} \right] dq$$

Here $\rho$, $M$, $g(r)$, $\Omega_0$, $F(q)$ and $S(q)$ be the number density, atomic mass, pair correlation function, atomic volume, energy wave number characteristic and the structure factor of the element, respectively. The expression for structure factor and pair correlation function is given in equation (2) and equation (3) respectively.

In the long-wavelength limit, the phonon dispersion curve shows an elastic behaviour. Hence, the longitudinal $\nu_L$ and transverse $\nu_T$ sound velocities are also calculated by

$$\omega_L \propto q \quad \omega_T \propto q, \quad \vdots \quad \omega_L = v_L q \quad \omega_T = v_T q$$

Various elastic properties are then determined by the longitudinal and transverse phonon frequencies.

The bulk modulus $B$, Poisson’s ratio $\xi$, modulus of rigidity $G$, Young’s modulus $Y$ and the Debye temperature $\theta_D$ are calculated using the expression below[7]

$$B = \rho \left( v_i^2 - \frac{4}{3} v_i^2 \right)$$

$$\xi = \frac{1 - 2(v_i^2 / v_i^2)}{2 - 2(v_i^2 / v_i^2)}$$

$$G = \rho v_i^2$$

$$Y = 2G(\xi + 1)$$

and

$$\theta_D = \frac{\hbar}{k_B} \left[ \left( \frac{9\rho}{4\pi} \right)^{1/3} \left( \frac{1}{v_i^3} + \frac{2}{v_i^3} \right)^{-1/3} \right]$$

where ‘h’ is Planck constant and $k_B$ is the Boltzmann constant.
3. Results and Discussion

Table 1: Input parameters and constants for Bi$_{50}$Zn$_{50}$ binary metallic glass

| T[K] | $Z_{\text{eff}}$ (au) | $\Omega_{\text{eff}}$ (a.u.$^3$) | $r_{\text{c eff}}$ (au) | $M_{\text{eff}}$ (a.m.u) |
|------|---------------------|-------------------------------|---------------------|-------------------|
| 793  | 173.351             |                               | 1.1613              |                   |
| 873  | 174.973             |                               | 1.1655              |                   |
| 1023 | 3.5                 |                               | 178.003             | 1.1721            |
| 1123 | 180.017             |                               |                    | 1.1766            |

The constant and parameters used in the present study of collective excitation are given in Table 1. In the fig 1 and fig 2 show the structure factors $S(q)$ and pair distribution functions $g(r)$ along with the experimental data [6] respectively. Good agreement with the experiment is observed for the structure factors and very good agreement is observed for pair correlation function at various temperatures. When temperature increases the position of the first peak points are shifted toward $q=0$. The present pair correlation function is used to compute the phonon modes and elastic properties for Bi-Zn binary alloy.

Figure 1. Structure factor, $S(q)$ for Bi$_{50}$Zn$_{50}$ alloys at different temperature along with Exp. data [6]
Figure 2. Pair distribution functions, \( g(r) \) for Bi\(_{50}\)Zn\(_{50}\) alloys at different temperature along with Exp. data [6].

Figure 3. Effective pair potential for Bi\(_{50}\)Zn\(_{50}\) binary metallic glass at various temperatures.
Our well established model potential [7,8] is used along with two different local field correction functions Hartree [9] and Farid et al [10] for the first time to produce effective pair potentials for Bi$_{50}$Zn$_{50}$ at various temperatures shown in fig 3. From figure 3 it is observed that position of the first minima is affected by the different types of screening functions along with various temperatures. The first minimum in the pair potential occurs nearly at same interatomic spacing. However, the magnitude of potential energy at first neighbour is greatly affected by type of screening as well as temperatures used in the system. The maximum depth in the pair potential in the present study is obtained due to F screening function. It is also noticed that the first zero for $V(r=r_0)$ due to two local field correction functions occurs at $r_0 \approx 12.39\,\text{Å}$ and $r_0 \approx 12.39\,\text{Å}$ for the H and F screening functions along with different temperatures, respectively. It is also observed that maximum depth position is not affected by the different temperatures. The oscillatory nature is also seen even at large $r$-region. Fig 4 shows the collective modes of present metallic glass. H gives the higher magnitude compared to F screening function and it is observed that the magnitude is increased as temperature increases. It is also observed that the position of the first minima approximately coincides with the first peak in the static structure factor of respective different temperatures for present alloy. We have not superimposed $S(q) \rightarrow q$ curve on $\omega \rightarrow q$ to avoid complication in the figures. It is also noticed that the related magnitude of first peak of PDC increases as a temperature increasers but the position of first peak is not affected by different screening functions. The first minimum in the longitudinal branch of the dispersion curve falls at a value $q \approx 2.68\,\text{Å}^{-1}$ and $q \approx 2.68\,\text{Å}^{-1}$ for H and F screening functions at different temperatures respectively. The first peak heights of the longitudinal and transverse phonon modes of this metallic glass are nearly the same at the different temperatures, so that, the dispersion curves of present alloys is found to be similar. Phonons of transverse branch undergo large thermal modulation due to anharmonicity of lattice vibrations in this branch. In the long wave length limit, the dispersion curves are linear and confirming characteristics of elastic wave.

![Figure 4. Longitudinal and Transverse phonon mode of Bi$_{50}$Zn$_{50}$ binary metallic glass at various temperatures.](image)
Table 2: Elastic properties of Bi$_{50}$Zn$_{50}$ binary metallic glass at various temperatures along with local field correction function

| properties | T=793K | T=873K | T=1023K | T=1123K | Cal. |
|------------|--------|--------|---------|---------|------|
| $v_L \times 10^5$ (cm/s$^2$) | 5.579 | 5.217 | 5.589 | 5.256 | 5.604 | 5.265 | 5.618 | 5.277 | -- |
| $v_T \times 10^5$ (cm/s$^2$) | 3.221 | 3.012 | 3.227 | 3.034 | 3.235 | 3.039 | 3.244 | 3.047 | -- |
| B$\times 10^{12}$ (dyne/cm$^2$) | 1.435 | 1.255 | 1.428 | 1.263 | 1.414 | 1.247 | 1.406 | 1.240 | 0.505 |
| G$\times 10^{12}$ (dyne/cm$^2$) | 0.861 | 0.752 | 0.857 | 0.758 | 0.848 | 0.748 | 0.843 | 0.744 | 0.275 |
| Y$\times 10^{12}$ (dyne/cm$^2$) | 2.152 | 1.882 | 2.143 | 1.893 | 2.120 | 1.871 | 2.109 | 1.860 | 0.70 |
| $\xi$ | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 | 0.25 | 0.29 |
| $\theta_D(K)$ | 361.1 | 337.7 | 360.5 | 339.0 | 359.4 | 337.6 | 358.9 | 337.1 | 224.5 |

Presently, calculated bulk modulus ($B_T$), modulus of rigidity ($G$), Poisson’s ratio ($\xi$), Young’s modulus ($Y$), Debye Temperature ($\theta_D$) and sound velocities are shown in Table 2. For this composition of Bi-Zn system, no experimental data of elastic constants are available in literature. As a result, we have average the elastic constants of pure Bi and Zn and the average values are shown in Table 2 along with the presently calculated values. It is observed in the present case that bulk modulus, modulus of rigidity and Young modulus are overestimate. The presently calculated values of elastic constants using H and F functions show overestimated with the average values. Thus, it is observed that proper local field correction function is necessary in order to estimate the elastic properties of metallic glasses like Bi-Zn.

4. Conclusion

Bi-Zn binary metallic glass is containing wide range of application in the field of technology and material science. So that, we conclude that results of structure factors and pair correlation functions found satisfactorily good agreement with available experimental data. The PDC generated from HB approach reproduces satisfactorily general characteristics of dispersion curves. The magnitude of longitudinal and transverses curves are increases as increases the temperatures. Present study of elastic properties will remain very useful to the set of theoretical data. This local model potential depends on effective core radius which is used here to describe the ion-electron interaction. The present study are also confirms the applicability of local model potential in the aforesaid properties. Our well known model potential along with H and F local field correction functions generates consistent results regarding the phonon modes of the binary metallic glasses.

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References
[1] B. Y. Thakore, S. G. Kambholja, P. H. Suthar, N. K. Bhatt and A. R. Jani 2010 Chin. Phys. Letts. 27 096203
[2] B. Y. Thakore, H. Dabhi, M. Joshi and A R Jani 2009 Phys. Scr. 79 0250007
[3] B. Y. Thakore, P. N. Gajjar and A. R. Jani 2000 Bull. Mat. Sci. 23 5
[4] A. M. Vora 2008 Rom. J. Phys. 53 517
[5] W. H. wang 2006 J. Apply.Phys. 99 093506
[6] H. Ueno, Y. Kawakita, K. Ohara, S. Tahara, S. Kohara, M. Itou and S. Takeda 2012 Proc. of the 5th European Conf. on neutron scattering J. Phys. Conf. Ser. 340 012081
[7] P. H. Suthar, P. N. Gajjar, B. Y. Thakore and A. R. Jani 2013 Proc. of the SciTech-2013, J Phys. Conf. Series 423 012030
[8] P. B. Thakore, P. N. Gajjar and A. R. Jani 2009 Pramana J. Phys. 72 1045
[9] W. A. Harrison 1967 Pseudopotential in the theory of metals W A Benjamine Publisher, New York
[10] B. Farid, V. Heine, G. E. Engel, I. J. Robertson 1993 Phys. Rev. B 48 11602
[11] N. W. Ashcroft and D. C. Langreth 1967 Phys. Rev. 156 685
[12] J. Hubbard and L. Beeby 1969 J. Phys. C 2 556