STRUCTURE AND DYNAMICS OF Ca70Zn30 METALLIC GLASS

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ABSTRACT

A new interatomic potential is computed for the two-component metallic Ca70Zn30 glass, treating it as a pseudo-one-component system. This potential is used to study the system's vibrational dynamics regarding localized excitations. The elastic and thermal transport properties are computed, knowing the sound velocities estimated from the elastic part of the dispersion curve. The obtained results depict a quite satisfactory description of the glassy system.

INTRODUCTION

Investigations for obtaining interatomic pair potentials for metallic alloy, glasses [1-4] have been attempted using the methods established for liquid metals [5,6]. An effective pair-potential was proposed [7] for $Ca_{70}Zn_{30}$ glass in Ashcroft form utilizing the concept of a Wigner-Seitz sphere, treating it as a pseudo-one-component system. Such a system has also been examined, treating glass as a supercooled liquid in static relaxation calculations [8].

This work was stimulated by the need to obtain realistic pair potentials for a binary metallic glass $Ca_{70}Zn_{30}$. Using these obtained potentials, the dynamics of an amorphous system have been studied in terms of localized longitudinal and transverse vibrations. The elastic and thermal properties of this glassy system have also been computed.

THEORETICAL DESCRIPTION

The effective pair-potential of the glass may be written in the form

$$V_{eff}(r) = \left(\frac{Z^{eff}}{r}\right)^2 - 2\left(\frac{(Z^{eff})^2}{\pi}\right)\int_0^\infty dQ \frac{Sin(Qr)}{Qr} F_N(Q) \quad \ldots (1)$$

With normalized energy wave number characteristic

$$F_N(Q) = \frac{Q^4\Omega^2}{16\pi^2 Z^2 e^4}\left[1 - \frac{1}{\varepsilon(Q)}\right]|W_b(Q)|$$

Eq.1 provides the interatomic potential between an effective pair of atoms, treating the binary metallic glass A_xB_{1-x} as a pseudo-one-component system of effective atoms. The mass and number density of effective atoms is

$$M^{eff} = xM_A + (1-x)M_B \quad \ldots (1)$$

$$\rho^{eff} = x\rho_A + (1-x)\rho_B$$

The Fourier transform of the Ashcroft [9] bare-ion pseudopotential is expressed as

$$W_b(Q) = -\frac{4\pi Z^{eff} e^2}{Q^2\Omega} Cos\,(Q.r_c^{eff}) \quad \ldots (2)$$

The dielectric response function $\varepsilon(q)$ is given as

$$\varepsilon(Q) = 1 - \frac{(4\pi e^2/Q^2)\chi(Q)}{1+(4\pi e^2/Q^2)\chi(Q).G(Q)} \quad \ldots (3)$$

The polarizability $\chi(Q)$ is expressed as

$$\chi(Q) = \frac{-mk_F}{\pi^2\hbar^2}\left[\frac{1}{2} + \frac{4k_F^2 - Q^2}{8k_F Q} ln\left|\frac{2k_F+Q}{2k_F-Q}\right|\right] \quad \ldots (4)$$

In Random Phase Approximation (RPA), the function G(Q) is called the local field function, accounting for the exchange and correlation among the conduction electrons. For the present study, we have chosen the function G(q) given by Hubbard and Sham [10]:

$$G(Q) = \frac{Q^2}{2\left[Q^2+\nu\left(K_F^{eff}\right)^2\right]} \quad \ldots (5)$$

$$\nu = \frac{2}{\left(1+0.153/\pi K_F^{eff}\right)}$$

$$K_F^{eff} = (3\pi^2 Z^{eff}\rho^{eff})^{1/3}$$

In the above expressions, r_c^{eff} is called the ionic core radius and is a disposable parameter. It is obtained using the relation:

$$x\frac{4}{3}\pi r_A^3 + (1-x)\frac{4}{3}\pi r_B^3 = \frac{4}{3}\pi r_{glass}^3 \quad \ldots (6)$$

Where r_A, r_B, and r_{glass} are the Wigner -Seitz radii of A, B, and glass, respectively. The Wigner-Seitz radius of the glass is related to the effective core radius by the relation [11]

$$r_C^{eff} = \frac{0.51 r_{glass}}{(Z^{eff})^{1/3}} \quad \ldots (7)$$

The localized vibrations expressed in terms of phonon eigen frequencies are meaningful quantities for studying the collective excitations in the system. The expressions for longitudinal and transverse phonon eigen frequencies in random phase approximation (RPA) are given as [12]

$$\omega_l^2(Q) = \omega_E^2\left[1 - \frac{3Sin(Q\sigma)}{Q\sigma} - \frac{6Cos(Q\sigma)}{Q\sigma} + \frac{8Sin(Q\sigma)}{Q\sigma}\right] \quad \ldots (8)$$

$$\omega_t^2(Q) = \omega_E^2\left[1 + \frac{3Cos(Q\sigma)}{Q\sigma} - \frac{3Sin(Q\sigma)}{Q\sigma}\right] \quad \ldots (9)$$

Where

$$\omega_E = \left[\frac{4\pi\rho^{eff}}{3M^{eff}}\int_0^\infty drr^2\, g_{eff}(r)\frac{\partial^2}{\partial r^2}V_{eff}(r)\right]^{1/2}$$

and "σ" is the hardcore diameter. The hardcore diameter of the alloy is obtained as [13]

$$\sigma = \frac{\pi}{6}[N_A\sigma_A^3 + N_B\sigma_B^3]$$

$$\eta = \frac{\pi}{6}\left(\frac{1}{\Omega}\right)(\sigma_{glass})^3$$

The longitudinal and transverse velocities of sound may be derived from the slope of the long wavelength limit of the dispersion relations. The isothermal bulk modulus may be expressed as

$B_r = \boldsymbol{\rho}(C_l^2 - 4/3C_t^2)$ …(10)

The elastic Debye temperature is given in terms of longitudinal and transverse velocities of sound by

$$\theta_D = \frac{h}{k_B}2\pi\left(\frac{9\eta}{4\pi}\right)^{1/2}\left[\frac{1}{C_l^2}+\frac{2}{C_t^2}\right]^{-1/3} \quad \ldots (11)$$

On the other hand, the averaged Debye temperature of a binary system is given [14] by

$$\frac{1}{\theta_D^2} = \frac{\rho_A}{\theta_{D_A}^2} + \frac{\rho_b}{\theta_{D_b}^2} \quad \ldots (12)$$

Where $\boldsymbol{\rho}_A$ and $\boldsymbol{\rho}_B$ are the atomic concentrations and Θ_A and Θ_B are the Debye temperature of the pure components.

RESULTS AND DISCUSSION

The effective pair potential for $Ca_{70}Zn_{30}$ glass is calculated using Eq.1. These potentials have been compared with those obtained from partial pair potentials [7] $V_{AA}(r)$, $V_{BB}(r)$, and $V_{AB}(r)$, and shown in Fig.1. Both the effective potentials are almost similar as far as the repulsive part is concerned. It can be observed from the figure that the present computed effective potential shows a slightly greater well depth moved towards the left as compared to the potential calculated from the results of Hafner [15]. The present computed potential shows significant oscillations and potential energy remains positive in the larger r-regions. The coulomb repulsive potential part seems to dominate the oscillations due to ion-electron-ion interaction. Hence, the present computed effective potential converges for r-∞ towards a value greater than zero.

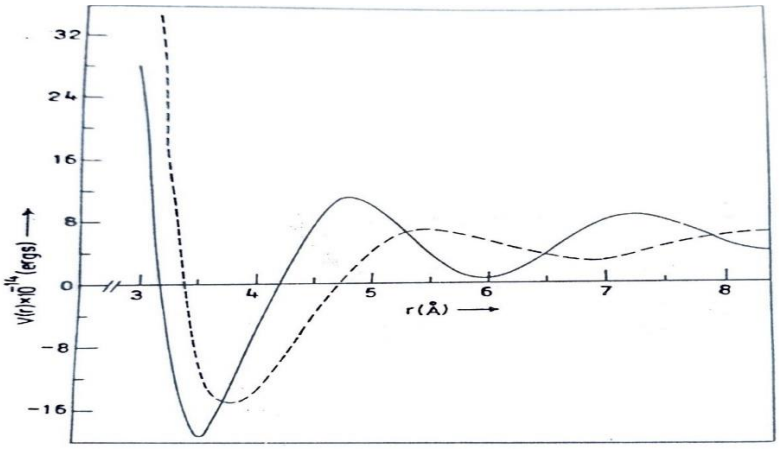

Fig.1: Effective pair-potential for Ca70Zn30 metallic glass: ▬▬ present results, --------results using partial pair potentials

The phonon eigen frequencies for the longitudinal and transverse phonon modes are computed using the obtained effective pair potentials with the help of Eqs. 8 and 9, and the results are shown in Fig.2. The longitudinal curve has the characteristic shape with a maximum and minimum. The low-wavevector transfer region depicts the characteristics of elastic waves. The first minimum in the ω-q curve for the longitudinal mode lies at approximately the same value of Q (=2.1A) at which the first peak of the static structure factor S(q) occurs [16]. Due to the non-availability of any experimental data on phonon dispersion for this glass, it has not been possible to compare the computed results with the experiment.

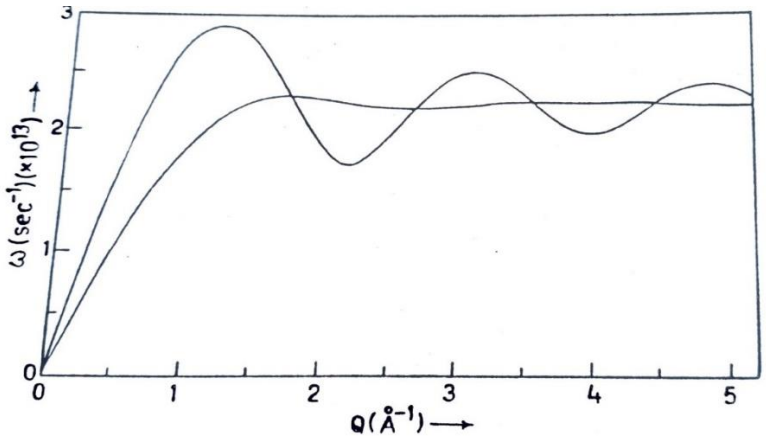

Fig.2: Present computed phonon dispersion results of $Ca_{70}Zn_{30}$ glass.

The accuracy of the results obtained for the phonon dispersion in the glass can be ascertained by the elastic and thermal properties obtained from the dispersion curves. In the long wavelength limit, the dispersion curves are linear and obey the relationship

$\omega_l = v_l Q$ and $\omega_t = v_t Q$

Where v_l and v_t are longitudinal and transverse sound velocities respectively. Using the values of the two velocities, elastic and thermodynamic properties like isothermal bulk modulus B_T and Debye temperature θ_D have been calculated for the system. The values of Debye temperature for pure components have been taken from Kittel [17]. The computed values are shown in the table.

Glassy system	v_l ($x10^5$Cm/sec)	v_t ($x10^5$Cm/sec)	B_T ($x10^{11}$Dynes/cm^2)	Averaged B_T ($x10^{11}$Dynes/cm^2)	θ_D(K)	Averaged θ_D (K)
$Ca_{70}Zn_{30}$	3.84	2.315	2.4 *(4.83% lower)*	2.49	251 *(7.2% higher)*	234

It can be observed that the results are of B_T and θ_D obtained using phonon spectra are in good agreement with the averaged value. The lower value of B_T shows the increase in compressibility i.e. softening of the material after glassification.

CONCLUSION

In brief, the new effective potential fairly describes the system's dynamics regarding w-q dispersion curves. Also, the calculated elastic and thermal properties depict the physical situation quite well.

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