PRAJÑĀ - **Journal of Pure and Applied Sciences Vol. 24 – 25 : 84 – 86 (2017)**
ISSN 0975 - 2595

PHONONS IN TERNARY METALLIC GLASS Cu-Ti-Zr

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ABSTRACT

In the present paper, results of our theoretical calculations of phonon frequencies and elastic constants for ternary metallic glass Cu-Ti-Zr are reported. Model potential formalism is used to compute the inter-ionic interactions. Phonon frequencies are calculated using the phenomenological approach of Hubbard and Beeby. The results are discussed in the light of experimental findings. Further, elastic constants are also estimated.

Keywords: Phonons, Ternary metallic glass, Elastic Constants.

INTRODUCTION

Synthesis of metallic glasses is challenging as metals easily crystallize upon solidification [1]. Further, bulk metallic glasses (BMGs) could also be synthesized [2]. Due to such advancement in synthesis, large amount of experimental and theoretical work on structural and elastic properties of metallic glasses is carried out by various researchers [3-12]. Copper based binary and bulk metallic glasses have shown exceptional physical properties like low mass, high strength, extraordinary plasticity etc [13]. Recently, various researchers have reported results of different physical properties of Cu-Zr based BMGs [14-16]. It is reported that the interionic interactions within hard sphere model system can be well described in terms of various forms of potentials like LJ potential, Morse potential, Dzugotov potential etc [1]. The most common feature in such potentials is that they show a first minimum at a nearest neighbor distances. Since such simple forms are insufficient to describe the interatomic interactions in metals [1], we need to use some realistic form of potential. In our recent work [5-7] we have adopted model potential formalism to describe the interatomic interactions in binary metallic glasses. Similar formulations have been used by other researchers also [15, 16]. Use of such a model potential within Wills-Harisson form is proved as reliable tool to describe the interatomic interactions in non-crystalline phase like metallic glasses, liquid metals and their alloys [5-7, 17, 18]. Recently, Han et al [10] have reported the liquid to glass transition in Cu Ti Zr glass forming system using molecular dynamics simulation. They have reported structural properties of this ternary system using Stillinger-Weber potential. However, the study of vibrational dynamics of this metallic glass is still missing and we thought it worthwhile to explore the vibrational properties of this system using a reliable theoretical tool. Thus, in the present work, we have calculated the phonon frequencies in ternary system Cu-Ti-Zr for its specific composition $Cu_{60}Ti_{20}Zr_{20}$ using model potential formalism in conjunction with phenomenological approach of Hubbard and Beeby [19]. The results are compared with experimental and other theoretical results, wherever available. The paper is organized as following. The next section deals with the theoretical formulation used to compute the interatomic interactions and phonon frequencies in ternary system. The results are discussed in section 3 and the findings are concluded in section 4.

METHODOLOGY

The effective ion-ion interaction in s-p bonded system is given as

$$V(r) = \frac{Z^2 e^2}{r} + \frac{2}{\pi}\int dq F(q)\exp(-iq\cdot r) \qquad (1)$$

In addition to above equation (1), while dealing with the transition metals, the *d band* correction is also important one [5-7]. In the present work, we have corrected the equation (1) by adding the *d band* correction terms as mentioned in [5-7]. $F(q)$ in (1) is an energy wave number characteristic. In the present study, we have considered the concept of "effective atom" to compute the dispersion curves. We have used Ashcroft's empty core model potential [20]. This model potential contains only one

parameter, the core radius. This parameter can be obtained through fitting specific quantities with the experimental ones. Instead of fitting procedure, we have calculated the core radius from the known Wigner-Seitz radius [5-7]. The exchange-correlation effects are incorporated through the forms of Ichimaru and Utsumi (IU) [21], as this form satisfy the compressibility sum rule in the long wavelength limit and can be applied to large range of densities. Along with effective pair potential, another important quantity is the pair correlation function of metallic glass. This function can be obtained through any experimental techniques or computer experiments like molecular dynamics simulation. Han et al [10] have obtained the pair correlation function of system of our interest using molecular dynamics simulation. In the present work, at this stage, we have adopted these values of Han et al [10] to compute the phonon frequencies.

Within the phenomenological approach of Hubbard and Beeby [19], the phonon frequencies are calculated using following set of equations (2) and (3);

$$\omega_l^2(q) = \omega_E^2\left[1 - \frac{3\sin(q\sigma)}{(q\sigma)} - \frac{6\cos(q\sigma)}{(q\sigma)^2} + \frac{6\sin(q\sigma)}{(q\sigma)^3}\right] \quad (2)$$

$$\omega_t^2(q) = \omega_E^2\left[1 + \frac{3\cos(q\sigma)}{(q\sigma)^2} - \frac{3\sin(q\sigma)}{(q\sigma)^3}\right] \quad (3)$$

Here, ω_E is the maximum phonon frequency and is given by following expression

$$\omega_E^2 = \frac{4\pi . n_{eff}}{3M_{eff}} \int_0^\infty g(r) r^2 V^{"}(r) dr \quad (4)$$

The $V_{eff}^{"}(r)$ in above expression (4) denotes the second order derivative of the effective pair potential and the upper limit in the integration is decided by the length of the $g(r)$ in the computation.

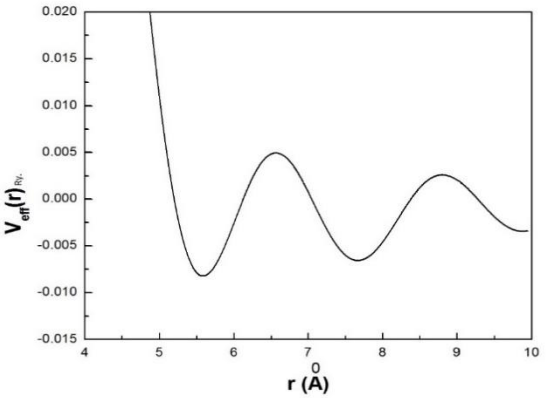

Figure 1. Effective pair potential in ternary metallic glass $Cu_{60}Ti_{20}Zr_{20}$.

The M_{eff} and n_{eff} are the effective atomic mass, effective number density respectively, and are calculated for present ternary system by weighted average over their concentration [5-6].

The M_A, M_B, n_A, n_B represents the atomic masses and number densities of the pure A and B components of the alloy respectively. Since in the long wavelength limit the phonon dispersion curves shows an elastic behavior which permit us to compute longitudinal and transverse sound velocities and other elastic constants [5-7].

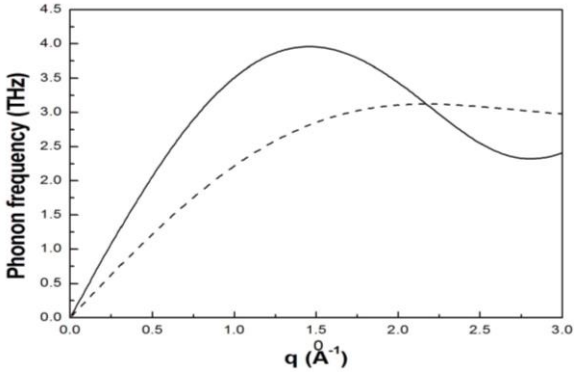

Figure 2. Longitudinal and Transverse Phonon Frequencies in $Cu_{60}Ti_{20}Zr_{20}$.

RESULTS AND DISCUSSION

In the present work, we have computed the effective pair potential using second order perturbation theory within Wills Harrison form along with *d band* correction terms. The computed pair potential is shown in Fig. 1. The existence of Friedel oscillations is clearly observed in the pair potential. The computed longitudinal and transverse phonon frequencies are shown in Fig. 2. It is seen that at large q values, momentum transfer is due to longitudinal phonons only. Transverse modes have very small role in momentum transfer as they undergo large thermal modulation. The first minimum in the longitudinal branch occurs at 2.8 $Å^{-1}$, near which the static structure factor should show principal peak. Hubbard-Beeby model considers each system as isotropic and hence it assumes the fix value of ratio of longitudinal to transverse sound velocity and hence fix value of Poisson's ratio i.e. 0.25. This is observed in our previous work [5-7]. Poisson's ratio is an important parameter in determining "*intrinsic plasticity*" of a material [1]. An et al [22] have noted that if the value of Poisson's ratio is less than 0.31, the material is brittle and its higher value is related to ductility of a material. Since, the presently used approach of Hubbard and Beeby avoids "*intrinsic plasticity*" of non-crystalline material, we can not put any concrete remark about brittleness or ductility of

Cu-Ti-Zr system. However, we can certainly say that the calculated longitudinal phonon frequency show all broad features of collective excitation in a metallic glass. From the long wavelength limit, we have calculated sound velocities of longitudinal and transverse branch and the results are 4.35 x 10^5 m/s and 2.51 x 10^5 m/s, respectively. Further, we have estimated bulk modulus of this system and the calculated value is 75.55 GPa. This value is in accordance with the hardness of metallic glass. In the study of Cu-Zr binary metallic glass also [5-7], a higher value of bulk modulus is observed, which indicates high hardness of Cu-Zr based metallic glasses.

CONCLUSION

In the present work, we have estimated the phonon frequencies and elastic constants of $Cu_{60}Ti_{20}Zr_{20}$ ternary metallic glass. This system has high hardness as observed through its bulk modulus. Modification in HB approach is required to correctly estimate the ductility and/or brittleness of a metallic glass.

ACKNOWLEDGEMENT

SGK is grateful to DAE-BRNS for Research Grant under a Major Research Project F. No. 39/14/29/2016-BRNS.

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