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Short Communication

Study of Phonon Dynamics of $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ Bulk Metallic Glass Using Pseudopotential

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In the present paper, the computations of the vibrational phonon frequencies of the longitudinal and transverse branches in a quaternary $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ bulk metallic glass (BMG) using simple Hubbard-Beeby (HB) model approach have been presented. Ashcroft's empty core model pseudopotential is utilized in conjunction with Hartree screening of conduction electrons with and without the inclusion of correlation effects by employing various forms of local field correction functions for the first time. The phonon frequency observations reproduce the typical features of the dispersing nature. Also, the thermodynamic and elastic properties of the said BMG are calculated through the elastic limit of the dispersion bends.

Keywords: Longitudinal and transverse phonon frequencies, Bulk metallic glass (BMG), Thermodynamic and elastic properties.

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1. INTRODUCTION

Bulk amorphous metallic alloys or bulk glassy metals or bulk metallic glasses (BMGs) signify new type of materials in the modern era of the materials science. They can be formed from the melt by its cooling with a sufficiently high cooling rate in order to avoid the crystallization in the temperature range between liquidus temperature and the glass transition temperature T_g. Meanwhile, much effort has been devoted to the progress of BMGs for both fundamental scientific research and industrial applications. As a result, many unique and useful properties of BMGs have been shown and studied significantly [1-4]. Looking to the applicability of the BMGs, the vibrational dynamics of $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ BMG is reported for the first time in the present article with the help of Ashcroft's empty core model pseudopotential [5]. Hartree (H) [1], Taylor (T) [1], Ichimaru-Utsumi (IU) [1], Farid *et al.* (F) [1] and Sarkar *et al.* (S) [1] local field correction functions are used for showing the screening dependency on the aforementioned properties. The phenomenological model proposed by Hubbard and Beeby (HB) [6] in the random phase approximation (RPA) is considered to make the phonon dispersion curve (PDC) with Wills-Harrison (WH) [7] approach of the pair potential. While, static and thermodynamic properties such as longitudinal sound velocity ν_L, transverse sound velocity ν_T, isothermal bulk modulus B_T, modulus of rigidity G, Poisson's ratio σ, Young's modulus Y and Debye temperature θ_D are also reported from the elastic limit of the dispersion curve.

2. COMPUTATIONAL METHODOLOGY

The interatomic pair potential is the fundamental component for learning the vibrational dynamics of BMGs. In the present work, the following equation is used to compute the pair potential [1-3, 7]:

$$V(r) = V_S(r) + V_b(r) + V_r(r). \quad (1)$$

The contribution from the *s*-electron to the interatomic pair potential $V_S(r)$ is obtained from the equation

$$V_S(r) = \left[\frac{Z_S^2 e^2}{r}\right] + \left(\frac{\Omega_0}{\pi^2}\right)\int F(q)\left[\frac{sin(qr)}{qr}\right]q^2 dq, \quad (2)$$

where Ω_0 is the total atomic volume of the monocomponent fluid. Here, the *s*-electron contribution, i.e. $Z_S \cong 1.5$, is obtained by mixing the partial *s*-density of states, which results from the self-consistent band structure computation for the entire 3*d* and 4*d* series.

The *d*-electrons, contributing to the interatomic pair potential, are described in terms of the number of *d*-electrons Z_d, *d*-state radii r_d and the nearest neighbor coordination number N as given below [1-3, 7]

$$V_b(r) = -Z_d\left(1-\frac{Z_d}{10}\right)\left(\frac{12}{N}\right)^{1/2}\left(\frac{28.06}{\pi}\right)\left(\frac{2r_d^6}{r^8}\right), \quad (3)$$

where $V_b(r)$ allows the Friedel-model band broadening to influence the transition metal cohesion

$$V_r(r) = Z_d\left(\frac{450}{\pi^2}\right)\left(\frac{r_d^6}{r^8}\right). \quad (4)$$

Here, $V_r(r)$ rises from the repulsion of the *d*-electron muffin-tin-orbital on different sites by the reason of their non-orthogonality. The effects of the *s*-band and *d*-band have been studied by Wills and Harrison (WH) [7]. Also, $F(q)$ is the energy wave-number characteristic in Eq. (2) given by [1-3]

$$F(q) = \frac{-\Omega_0 q^2}{16\pi}\left|W_B(q)\right|^2 \frac{\left[\varepsilon_H(q)-1\right]}{\left\{1+\left[\varepsilon_H(q)-1\right]\left[1-f(q)\right]\right\}}, \quad (5)$$

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where $f(q)$ is the local field correction function and $W_B(q)$ is the Ashcroft's empty core model pseudopotential [5]. For present BMG, the model pseudopotential parameter r_C is calculated from the well-known formula [1, 2]

$$r_C = \left[\frac{(0.51)r_S}{Z^{1/3}}\right], \quad (6)$$

where r_S is the Wigner Seitz radius of the BMG.

The theory of computing the vibrational dynamics of BMGs, the RPA model proposed by Hubbard and Beeby (HB) [6], is used in the present work. The notations for longitudinal ω_L and transverse ω_T phonon frequencies are computed from

$$\omega_L^2(q) = \omega_E^2\left[1 - \frac{\sin q\sigma}{q\sigma} - \frac{6\cos q\sigma}{(q\sigma)^2} + \frac{6\sin q\sigma}{(q\sigma)^3}\right] \quad (7)$$

and

$$\omega_T^2(q) = \omega_E^2\left[1 - \frac{3\cos q\sigma}{(q\sigma)^2} + \frac{3\sin q\sigma}{(q\sigma)^3}\right] \quad (8)$$

with

$$\omega_E^2 = \left(\frac{4\pi\rho}{3M}\right)\int_0^\infty g(r)V''(r)r^2dr\,. \quad (9)$$

Here, M and ρ are the atomic mass and density of the BMGs, while $V''(r)$ is the second derivative of the interatomic pair potential and $g(r)$ is the pair correlation function, respectively. The elastic and thermodynamic properties such as viz. longitudinal sound velocity v_L, transverse sound velocity v_T, isothermal bulk modulus B_T, modulus of rigidity G, Poisson's ratio σ, Young's modulus Y and Debye temperature θ_D are calculated directly from the elastic boundary of the dispersion curves [1-3].

3. RESULTS AND DISCUSSION

The inputs utilized in the current calculation are tabulated in Table 1.

Table 1 – Input parameters and constants

Z	N	M (amu)	Ω_0 (au)^3	Z_d	r_C (au)
2.20	12	79.01	105.84	6.70	1.3074

The computed pair potentials of $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ BMG are displayed in Fig. 1, which clarifies that the incidence of the various local field correction functions hardly changes the nature of the pair potentials, except around the first minima. The well depth is slightly rising due to the effect of various local field correction functions compared to H-function. The first zero position of the pair potentials is shown at $r = r_0 = 3.17$ au for T-function and those for others are shown at $r = r_0 = 3.6$ au. Thus, the occurrence of the exchange and correlations on the $V(r = r_0)$ is found significantly in the nature of the pair potential, while the potential well width increases compared to H-screening function. The well depth of currently computed pair potentials is shifted to the left direction. Also, it can be noted that the Coulomb repulsive potential part controls the fluctuations due to ion-electron-ion interactions, which displays the flattened shape of the potential after $r \approx 10$ au, which converged towards a finite value nearer to zero in repulsive region. Only oscillatory nature is observed for T- and F-functions because of ion-electron-ion interaction effect, which shows short-range order oscillation.

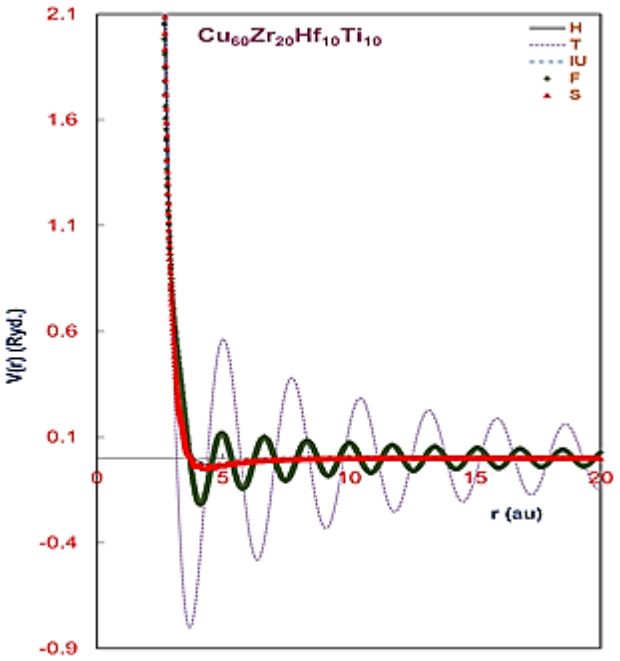

Fig. 1 – Pair potentials for $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ BMG

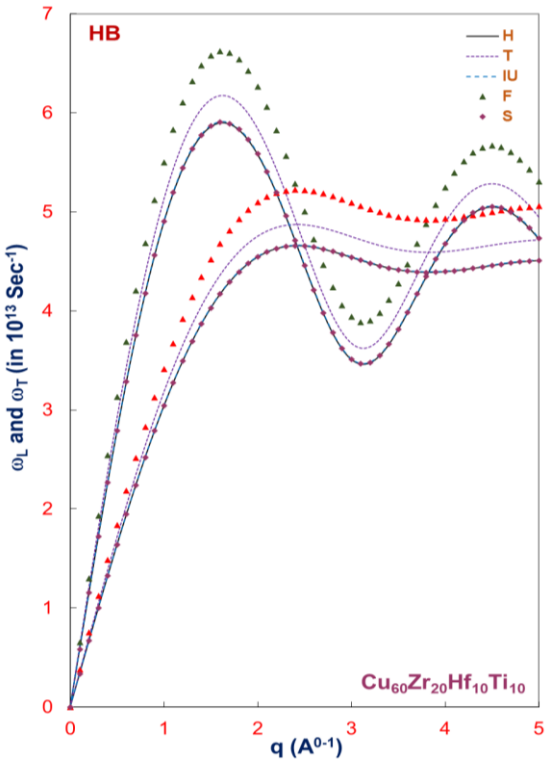

Fig. 2 – Phonon dispersion curves for $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ BMG

The screening dependences of phonon dispersion curves with longitudinal and transverse branches for $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ BMG computed using HB approach are shown in Fig. 2. It is observed that the present outcomes of the phonon branches due to T, IU and S-screening functions are seeing between H- and F-screening functions.

Table 2 – Thermodynamic and elastic properties

SCR	H	T	IU	F	S
$\nu_L \times 10^5$ cm/s	5.82	6.09	5.82	6.53	5.82
$\nu_T \times 10^5$ cm/s	3.36	3.51	3.36	3.77	3.36
$B_T \times 10^{11}$ dy/cm^2	15.75	17.25	15.79	19.83	15.77
$G \times 10^{11}$ dy/cm^2	9.45	10.35	9.47	11.90	9.46
σ	0.25	0.25	0.25	0.25	0.25
$Y \times 10^{11}$ dy/cm^2	23.63	25.87	23.69	29.74	23.65
θ_D (K)	444.13	464.73	444.66	498.25	444.31

The first minima in the longitudinal mode are made from the place almost around $q \approx 3.1$ Å^{-1} for most of the local field correction functions. Also, the first minima of the longitudinal branch are displayed at higher q-values. The lowest minima in the longitudinal mode clarify accuracy and constancy of the interatomic pair potential. Such reproductions were also detected in the transverse branch. Besides, it is detected that the fluctuations are further projecting in the longitudinal phonon branches with respect to the transverse branches because of the presence of joint excitations at higher momentum transfer owing to the longitudinal phonons and the ambiguity of the transverse phonons due to the anharmonicity of the atomic vibrations in the BMG system. Although, in the higher wave vector region damping of phonons governs the transverse mode which shows the fluid type nature i.e. monoatomic of the amorphous system. In transverse mode, the phonon frequencies rise with the wave vector q and then saturate at $q \approx 2.5$ Å^{-1}, which is found in connection with Thorpe model [8]. The transverse phonons are absorbed for frequencies higher than the lowest eigenfrequencies of the largest band.

Additionally, the elastic and thermodynamic properties computed from the elastic limit of the phonon dispersion curves are given in Table 2. The percentile impact of various screening functions with static H-function is found between 0-25.85 %. It is observed that the screening functions play a dynamic role in the estimation of the thermodynamic and elastic properties of BMG. The experimental or theoretical data are not available for such BMG for further comparison.

4. CONCLUSIONS

The computed data of phonon dispersion and their related properties using HB approach are exposed reliable fallouts. The screening effects are also observed in the present work by using various local field correction functions. Because of non-availability of experimental figures of such properties, present results formed very valuable information of particular BMG for additional researches.

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Вивчення динаміки фононів об'ємного металевого скла $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ з використанням псевдопотенціалу

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У статті представлено обчислення коливальних частот фононів поздовжньої та поперечної гілок у чотирикомпонентному об'ємному металевому склі (BMG) $Cu_{60}Zr_{20}Hf_{10}Ti_{10}$ з використанням простого модельного підходу Хаббард-Бібі. Псевдопотенціал моделі Ешкрофта з порожнім ядром застосовується спільно з екрануванням Хартрі електронів провідності з та без включення кореляційних ефектів, вперше використовуючи різні форми корегувальних функцій локального поля. Спостереження фононної частоти відтворюють типові риси дисперсійного характеру. Крім того, термодинамічні та пружні властивості згаданого BMG розраховуються через межу пружності дисперсійних вигинів.

Ключові слова: Поздовжні та поперечні фононні частоти, Об'ємне металеве скло (BMG), Термодинамічні та пружні властивості.