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Phonon Dynamics of Bulk Metallic Glass Using Takeno-Goda Approach

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Abstract. In the present article, the phonon dynamics of $Pd_{39}Ni_{10}Cu_{30}P_{21}$ bulk metallic glass (BMG) using Show's optimized model pseudopotential at room temperature are reported. The theoretical effective atom model (EAM) with Wills-Harrison (WH) approach are utilized for the computation of the interatomic pair potential (PP) and pair correlation function (PCF), respectively. Also, the phonon dispersion curves and their related static and thermodynamic properties are computed through Takeno-Goda (TG) model. The screening dependency on the aforesaid properties are studied by using different forms of the local field correction functions.

Keywords: Pair potential, Bulk Metallic Glasses (BMG), Phonon Dispersion Curves, Thermodynamic and Elastic Properties.

1. Introduction

Bulk metallic glasses (BMGs) are the metastable solids without the long-range order existing in the crystals. Well-arranged metallic microstructures formed by the single crystal grains of varying size are the basic building blocks of any metallic material. Metal alloys are usually found by melting and subsequent solidification; the particular cooling path and further thermal treatments are ultimately responsible of the crystallization procedure and final metallic microstructure which, in turn, define the mechanic response. Unlike crystalline alloys, the bulk metallic glasses (BMGs) are found by fast freezing below the crystallization temperature. It prevents regular crystallization and thus the material keeps the structure of the precursor liquid; hence, the bulk metallic glasses are thus solid materials with liquid-like structure at the atomic level. This non-crystalline structure makes the BMGs more resistant to permanent distortion than their crystalline nature by factors of 2 or 3 and tougher than ceramics [1-7]. Considering the applicability of the bulk metallic glasses, presently we report the vibrational dynamical study of $Pd_{39}Ni_{10}Cu_{30}P_{21}$ BMG with the help of well-known Shaw's constant core model potential [8]. Previously, we have reported phonon properties of such BMG using Hubbard-Beeby (HB) approach and found successful [7]. In connection with our previous study, such work is provided the linkage between the applications of two different theoretical phonon models. The important properties viz. longitudinal and transverse sound velocity; v_L and v_T bulk modulus B_T, Poisson's ratio σ, rigidity modulus G, Young's modulus Y and Debye temperature θ_D are calculated. Five different types of local field correlation functions given by Hartree (H) [9], Taylor (T) [10], Ichimaru-Utsumi (IU) [11], Farid *et al.* (F) [12] and Sarkar *et al.* (S) [13] are used for studying the screening dependency on the aforesaid studies. The

phonon dispersion curves (PDCs) are obtained by using a theoretical model proposed by Takeno and Goda (TG) [14, 15]. Further, the Wills-Harrison (WH) [16] model is used to compute the pair potential as a very important part of the PDC.

2. Computational Method

The expression of the presently computed pair potential through Wills-Harrison (WH) [1-7, 16] model for BMG is as follows,

$$V(r) = V_S(r) + V_b(r) + V_r(r). \tag{1}$$

Where, the first term of the above equation $V_S(r)$ is actually, the $s-$electron contribution and it can be represented as,

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

Here, Ω_0 is used to represent the atomic volume of the BMG. The self-consistent band structure calculation can provide the partial $s-$density of states which can be used to obtain Z_S [1-7, 16]. The term $F(q)$ under integration in the above equation can be written as [1-7, 16]

$$F(q) = \frac{-\Omega_0 q^2}{16\pi} |W_B(q)|^2 \frac{[\varepsilon_H(q) - 1]}{\{1 + [\varepsilon_H(q) - 1][1 - f(q)]\}}. \tag{3}$$

In the present calculation, the model potential $W_B(q)$ proposed by Shaw [8] is used. The form of the potential is as follows [8],

$$W_B(q) = \frac{-8\pi Z}{q^2 \Omega_0} \left[\frac{\sin(qr_C)}{qr_C} \right]. \tag{4}$$

$\varepsilon_H(q)$ and $f(q)$ are the Hartree dielectric screening function [9] and the exchange and correlation function, respectively. The model potential parameter is a single parametric potential and the potential parameter r_C used in the present potential is calculated from following expression [1-7]:

$$r_C = \left[\frac{0.51 r_S}{(Z)^{1/3}} \right]. \tag{5}$$

Where r_S is the Wigner-Seitz radius of the BMG. And Z_d is the number of $d-$electron that

contributes to the pair potential and the nearest-neighbor coordination number N_C and the d – state radii r_d are used as follows:

$$V_b(r) = -Z_d\left(1-\frac{Z_d}{10}\right)\left(\frac{12}{N_C}\right)^{\frac{1}{2}}\left(\frac{28.06}{\pi}\right)\frac{2r_d^3}{r^5}, \tag{6}$$

and

$$V_r(r) = Z_d\left(\frac{450}{\pi^2}\right)\frac{r_d^6}{r^8}. \tag{7}$$

The theory proposed in the model of Takeno and Goda (TG) [14, 15] is used for computing the phonon dynamics of BMG. The expressions for two components of the phonon frequencies i.e. longitudinal (ω_L) and transverse (ω_T) as per TG model are computed from [14, 15]

$$\omega_L^2(q) = \left(\frac{4\pi\rho_{eff}}{M_{eff}}\right)\int_0^\infty drg(r), \tag{8}$$

and

$$\omega_T^2(q) = \left(\frac{4\pi\rho_{eff}}{M_{eff}}\right)\int_0^\infty drg(r). \tag{9}$$

$V''(r)$ is the second derivative of the pair potential. Some of the related properties such as longitudinal and transverse sound velocity v_L and v_T bulk modulus B_T, Poisson's ratio σ, rigidity modulus G, Young's modulus Y and Debye temperature θ_D are also covered under the study.

3. Results and discussion

The input parameters and other related constants used in the present calculation are tabulated in Table 1.

Table 1. Input parameters and constants.

BMG	Z	N_C	M (amu)	Ω_O (au)3	Z_d	r_C (au)
$Pd_{39}Ni_{10}Cu_{30}P_{21}$	2.33	9.48	72.93	100.94	7.02	0.8382

The calculated pair potentials of $Pd_{39}Ni_{10}Cu_{30}P_{21}$ BMG are obtained as shown in Figure 1, which explicates that almost no change is found in the nature of the pair potential by changing the local field correction functions except at or near the first minima. The slight increase is found in the depth of the well due to impact of various local field correction functions as compared to $H-$function. The first zero location in the Figure 1 arises at $r=r_0=2.5$ au. Thus, the presence of the exchange and correlations on the $V(r=r_0)$ is not found significantly. But, the width of the potential well is more than that of the $H-$screening function. The leftward shift of the well depth of pair potential is observed. The flatness in the plot after $r\approx 10$ au is shown because of the gradually vanishing of the oscillation arise due to ion-electron interaction by Coulombian repulsion of potential.

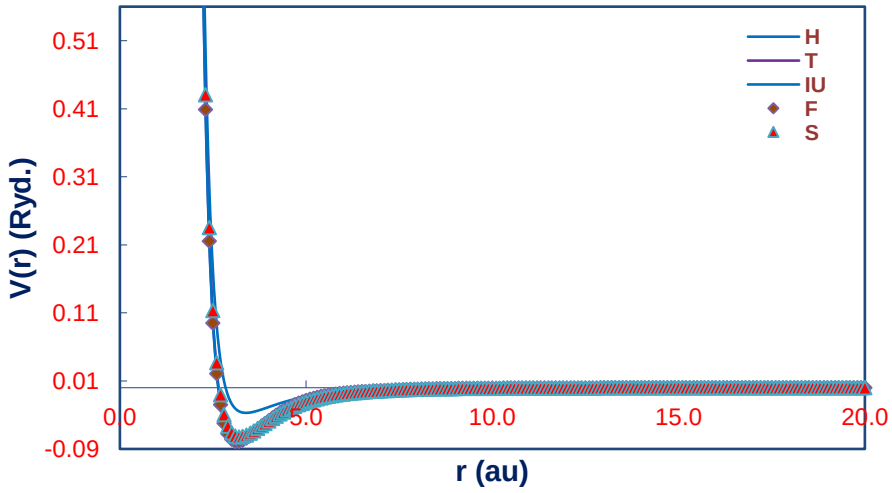

Fig. 1. Pair Potentials for $Pd_{39}Ni_{10}Cu_{30}P_{21}$ Bulk Metallic Glass.

The longitudinal and transverse branches of the phonon dispersion curves with the five screening functions for $Pd_{39}Ni_{10}Cu_{30}P_{21}$ BMG calculated using TG approach are exposed in Figure 2. It is to be observed that the present fallouts of the phonon modes obtained with the correction functions due to H, IU and $F-$function are positioned between those due to $S-$ and $T-$functions. The first minimum in the longitudinal branch is originated from the place at 2.7Å^{-1} for H, 2.7Å^{-1} for T, 2.8Å^{-1} for IU, F and $S-$local field correction functions. Also, the first minimum of longitudinal branch shows at higher $q-$values. The lower minima in the longitudinal branch explains the exactness and permanency of the pair potential. Such reflections are also seen in transverse mode. Apart from this, it is also observed that, the oscillations in case of longitudinal mode are more prominent as compare to the transverse mode. It is because of two reasons: out of which the one is the presence of collective excitations at higher momentum transfer owing to the longitudinal phonons only and another one is the uncertainty of the transverse phonons due to the inharmonicity of the atomic vibrations in the BMG systems. In the higher $q-$region, damping of phonons governs the transverse mode which shows the fluid type nature i.e. monoatomic of the amorphous system. Present results

show the analogy with the Thorpe model [17] as particularly in transverse branch only, the phonon frequencies rise with the values of q and after that the saturation is obtained at $q \approx 2.0 \mathring{A}^{-1}$. The transverse phonons are absorbed for frequencies higher than the lowest eigen frequencies of the largest cluster.

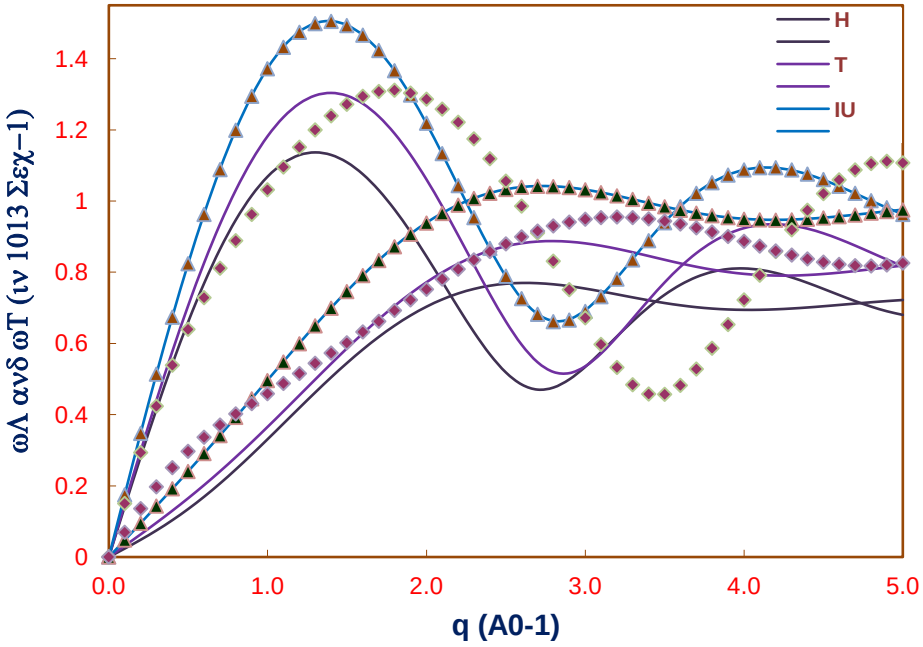

Fig. 2. Phonon Dispersion Curves for $Pd_{39}Ni_{10}Cu_{30}P_{21}$ Bulk Metallic Glass.

Furthermore, the thermodynamic and elastic properties of studied BMG estimated from the elastic limit of the phonon dispersion curves are tabulated in Table 2. The percentile influence of various screening functions with static H – function is found between $0.92\% - 91.94\%$. It is understood that the screening scheme plays a vital role in the estimation of the thermodynamic and elastic properties of BMGs. The experimental or theoretical data are not available for such BMG for further comparison.

Table 2. Thermodynamic and Elastic properties of $Pd_{39}Ni_{10}Cu_{30}P_{21}$ Bulk Metallic Glass.

SCR	υ_L**x10^5 cm/s**	υ_T**x10^5 cm/s**	B_T **x 10^{11} dyne/cm2**	G **x 10^{11} dyne/cm2**	σ	Y **x 10^{11} dyne/cm2**	θ_D **(K)**
H	1.2825	0.2356	1.2713	0.0449	0.4825	0.1332	32.5720
T	1.3645	0.3156	1.3995	0.0806	0.4717	0.2372	43.5787
IU	1.6117	0.4747	1.8591	0.1824	0.4525	0.5298	65.4115
F	1.6083	0.4733	1.8518	0.1813	0.4526	0.5267	65.2178
S	1.4625	0.7018	1.1245	0.3737	0.3504	1.0092	107.3437

4. Conclusion

The presently computed data of phonon dispersion curves and their related properties through TG approach are shown consistent results for studied BMG. The screening effects are also observed from the present study by employing different types of local field correction functions in all the properties. Non-availability of experimental data of the various properties of $Pd_{39}Ni_{10}Cu_{30}P_{21}$ bulk metallic glass (BMG), such results are form a very useful data set for the particular BMG for further investigations either theoretically or experimentally.

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