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VIBRATIONAL DYNAMICS OF PD-NI-P BULK METALLIC GLASSES: A LOCAL PSEUDOPOTENTIAL STUDY

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Abstract. *In this paper, phonon frequencies and elastic constant of three different concentrations of $Pd_xNi_{1-x}P_{20}$ ($Pd_{64}Ni_{16}P_{20}$, $Pd_{40}Ni_{40}P_{20}$, and $Pd_{16}Ni_{64}P_{20}$) bulk metallic glasses are calculated using approach of Hubbard-Beeby (HB) and Takeno-Goda (TG). We used our well established local model potential. The Hartree (H), Farid, et al. (F), and Sarkar et al (S) local field correlation functions are employed to study the effect exchange and correlation on the collective dynamics of Pd-Ni-P bulk metallic glasses. The results are reported for pair potentials, phonon dispersion curves, and elastic properties viz: coefficient of elasticity B_T, modulus of rigidity G, Poisson's ratio ξ, Young's modulus Y, Debye temperature θ_D. The calculated results of elastic constants are agreed with other theoretical and available experimental data.*

Keywords: vibrational dynamics; bulk metallic glass; elastic properties; pseudopotential; local field correction functions.

Classification numbers: 63.20kr; 71.23cq; 73.20Mf.

I. INTRODUCTION

From the literature survey it is found that, the metal-metalloid Pd-based bulk metallic glass was found before three decades [1–8] and known to be the first bulk metallic glass (BMG). In early 1990s, Turnbull and co-workers [4, 5] were successful in preparing the centimeter sized Pd–Ni–P metallic glass slab. Due to the high cost of Pd metals, initially the research work was only academic. But the development and related research work on latest BMG systems and its

usefulness in physics, chemistry and engineering fields has reworked interested in studying Pd-Ni-P glass. Because of excellent physical properties and its glass forming ability, it is useful in metallurgical and industrial application [4–9]. It is also necessary to understand thermodynamics, transport, and other properties of condensed systems [10–12]. There are two simple ways to compute frequencies in the BMG. First one is the approach due to Hubbard and Beeby [13], who used random phase approximation and conceptualized that the maxima in the product of $g(r)$ and $d^2V(r)/dr$ occur near to the hard core radius [14]. The second approach is due to Takeno and Goda [15, 16], who used many body correlation functions of atoms and interatomic potential. Hosokawa *et al.* [1] have derived phonon excitation for $Pd_{40}Ni_{40}P_{20}$ by inelastic X-ray scattering. Wang [6, 7] has reported the thermodynamics and elastic properties of the ternary system for Pd-Ni-P on specific three combinations viz; $Pd_{16}Ni_{64}P_{20}$, $Pd_{40}Ni_{40}P_{20}$, $P_{64}P_{16}P_{20}$ bulk metallic glasses (BMGs) using the ultrasound method. There are few theoretical investigations on Pd-based bulk metallic glasses where researchers have used these approaches to study vibrational dynamics [8]. In this paper we report the phonon dispersion curves (PDC) and elastic properties for $Pd_{16}Ni_{64}P_{20}$, $Pd_{40}Ni_{40}P_{20}$ and $P_{64}P_{16}P_{20}$ BMGs using (1) Hubbard- and Beeby [14] and (2) Takeno and Goda (TG) approaches [15,16]. Our well established model potential [17,18] with the exchange and correlation functions due to Hartree (H) [19], Farid *et al.* [20], Sarkar *et al.* [21] is used in the present investigations for Pd-Ni-P bulk metallic glasses.

II. COMPUTATIONAL METHOD

II.1. Model potential

The selection of model potential is an important role as it describes the motion of valance electrons in a metal. For the present study, we have used single parametric local model pseudopotential of the following form [17, 18].

$$\begin{aligned} V^{ion}(r) &= 0, \quad \text{for } r < r_c \\ V^{ion}(r) &= \frac{-Ze^2}{r} + \frac{Ze^2}{r}\exp\left(\frac{-r}{r_c}\right), \text{ for } r \geq r_c, \end{aligned} \tag{1}$$

where Z is the valency, e be the electronic charge and r_c is the model potential parameter.

This well tested model potential [17, 18] is the improved form of Ashcroft's empty core model potential [17]. The potential is continuous in r- space and in comparison with Ashcroft empty core model potential, we have introduced $\frac{Ze^2}{r}\exp\left(\frac{-r}{r_c}\right)$ as a repulsive term outside the corsece which helps in making damping quicker than only Coulomb potential. Moreover, the inclusion of the repulsive term outside the core makes the effective core smaller than the ionic radius of the free electron. In the reciprocal space, the corresponding bare-ion form factor of the present model potential is given by [18],

$$V_b(q) = \frac{-4\pi Z_{eff}e^2}{\Omega_{0eff}q^2}\left[\cos\left(qr_{ceff}\right) - \frac{\exp(-1)\left(qr_{ceff}\right)}{\left(1+q^2r_{ceff}^2\right)}\left\{\sin\left(qr_{ceff}\right) + qr_{ceff}cos\left(qr_{ceff}\right)\right\}\right]. \tag{2}$$

Here Z_{eff}, Ω_{0eff}, q, e and r_{ceff} is the valency, atomic volume, wave vector, charge of the electron and the parameter of the potential, respectively.

II.2. Pair Potential

In the present work, the Wills-Harrison (WH) [22] method is used to compute the pair potential. The relation used is [8, 22]

$$V(r) = Vs(r) + \left(-Z_d\left(1-\frac{Z_d}{10}\right)\left(\frac{12}{N_c}\right)^{\frac{1}{2}}\left(\frac{28.06}{\pi}\right)\frac{2r_d^3}{r^5}\right) + Z_d\left(\frac{450}{\pi^2}\right)\frac{r_d^6}{r^8}. \tag{3}$$

Here, Z_d is the contribution of d-electron to the pair potential and expressed in terms of the number of d-electron, r_d is the radius of d-orbital and N_C is the nearest-neighbour coordination number [8, 12, 13].

Also,

$$Vs(r) = \left(\frac{Z_{eff}^2 e^2}{r}\right) + \frac{\Omega_{0eff}}{r}\int dq F_{eff}(q)\left[\frac{\sin(qr)}{qr}\right]q^2. \tag{4}$$

Here $F_{eff}(q)$ is the effective wave number characteristics.

The other important integral in the study of phonon dispersion curves is the pair correlation function $g(r)$. The pair correlation function is computed by

$$g(r) = \exp\left[\left(\frac{-V''_{eff}(r)}{k_B T}\right) - 1\right]. \tag{5}$$

The energy wave number characteristics, $f_{eff}(q)$ appearing in Eq. (4) is written as

$$F_{eff}(q) = \left(\frac{-\Omega_{0eff}}{16\pi}\right)\left|V_b^{eff}(q)\right|\frac{\left[\varepsilon_H^{eff}(q)-1\right]}{\left\{1+\left[\varepsilon_H^{eff}(q)-1\right]\left[1-f_{eff}(q)\right]\right\}}. \tag{6}$$

Here, $V_b^{eff}(q)$ is the effective bare ion local pseudo potential as given in Eq. (1), $\varepsilon_H^{eff}(q)$ is the Hartree dielectric response function [12] and $f_{eff}(q)$ is the local field correction function that presents the exchange and correction effects. The three exchange and correlation functions of Hartree (H) (without exchange and correlation effect) [19], Farid *et al.* (F) [20] and Sarkar *et al.* (S) [21] are considered for the examination of relative effect of exchange correction on PDCs and elastic properties of Pd-Ni-P metallic glasses.

II.3. Photon Dispersion Curves and Elastic Constants Equations

In the Hubbard and Beeby [14] approach, the longitudinal and transverse phonon frequencies are computed using [8, 14, 18];

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

$$\omega_T^2(q) = \omega_E^2\left[1+\frac{3\cos(q\sigma)}{(q\sigma)^2}-\frac{6\sin(q\sigma)}{(q\sigma)^3}\right]. \tag{8}$$

Here, ω_E represents the maximum phonon frequency and is given by

$$\omega_E = \frac{4\pi n_{eff}}{3M_{eff}} \int_0^\infty g(r) r^2 V_{eff}^{"}(r) dr. \tag{9}$$

Here, ρ, M_{eff}, $g(r)$, Ω_{0eff}, and $F_{eff}(q)$ are the number density, atomic mass, pair correlation function, atomic volume and energy wave number characteristic, respectively.

Moreover, in the approach of Takeno Goda (TG) [15,16] for longitudinal phonon frequency ω_L and transverse phonon frequency ω_T are [15, 16]

$$w_L^2(q) = \frac{4\pi\rho}{M} \int_0^\infty dr g(r) \left[\begin{array}{c} rV'(r)\left(1 - \frac{\sin(qr)}{qr}\right) + \left\{r^2V''(r) - rV'(r)\right\} \\ \times \left\{\frac{1}{3} - \frac{\sin(qr)}{qr} - 2\frac{\cos(qr)}{(qr)^2} + 2\frac{\sin(qr)}{(qr)^3}\right\} \end{array} \right], \tag{10}$$

$$w_T^2(q) = \frac{4\pi\rho}{M} \int_0^\infty dr g(r) \left[\begin{array}{c} rV'(r)\left(1 - \frac{\sin(qr)}{qr}\right) + \left\{r^2V''(r) - rV'(r)\right\} \\ \times \left\{\frac{1}{3} + \frac{\cos(qr)}{(qr)^2} - \frac{\sin(qr)}{(qr)^3}\right\} \end{array} \right]. \tag{11}$$

The elastic nature in the phonon modes has been seen in the long-wavelength limit, hence, the longitudinal ν_l and transverse ν_t sound velocities are also computed by HB and TG approaches, respectively [12, 13]

$$v_l(HB) = \omega_E \sigma \left(\frac{3}{10}\right)^{1/2}, \tag{12}$$

$$v_t(HB) = \omega_E \sigma \left(\frac{1}{10}\right)^{1/2}, \tag{13}$$

where σ is the hard sphere diameter.

$$v_l(TG) = \left[\left(\frac{4\pi\rho}{30M}\right) \int_0^\infty dr r^3 g(r) \left\{3rV_{eff}''(r) + 4V_{eff}'(r)\right\}\right]^{\frac{1}{2}}, \tag{14}$$

$$v_t(TG) = \left[\left(\frac{4\pi\rho}{30M}\right) \int_0^\infty dr r^3 g(r) \left\{rV_{eff}''(r) + 4V_{eff}'(r)\right\}\right]^{\frac{1}{2}}. \tag{15}$$

The bulk modulus B_T, Poisson's ratio ξ, modulus of rigidity G, Young's modulus Y and the Debye temperature θ_D are studied with the following equation [12, 13, 18],

$$B_T = \rho\left(v_l^2 - \frac{4}{3}v_t^2\right), \tag{16}$$

$$G = \rho v_t^2, \tag{17}$$

$$\xi = \frac{1 - 2\left(v_t^2/v_l^2\right)}{2 - 2\left(v_t^2/v_l^2\right)}, \tag{18}$$

$$Y = 2G(\xi + 1) \tag{19}$$

and

$$\theta_D = \frac{h}{k_B}\left[\left(\frac{9\rho}{4\pi}\right)^{1/3}\left(\frac{1}{v_l^3}+\frac{2}{v_t^3}\right)^{-1/3}\right], \tag{20}$$

where ρ is the isotropic density of the solid, 'h' is Planck constant and k_B is the Boltzmann constant.

III. RESULTS AND DISCUSSION

Table 1. Input parameters and constants.

Parameters	$\mathbf{Z_{eff}}$	$\mathbf{\Omega_{0eff}(a.u)}$	$\mathbf{r}_{ceff\,(a.u)}$	$\mathbf{Z_d}$	$\mathbf{r_{d(a.u)}}$	$\mathbf{N_c}$
$Pd_{16}Ni_{64}P_{20}$	2.52	80.24	1.003	7.50	1.143	10.4
$Pd_{40}Ni_{40}P_{20}$	2.40	86.63	1.074	7.20	1.247	10.4
$Pd_{64}Ni_{16}P_{20}$	2.28	93.01	1.310	6.96	1.351	10.4

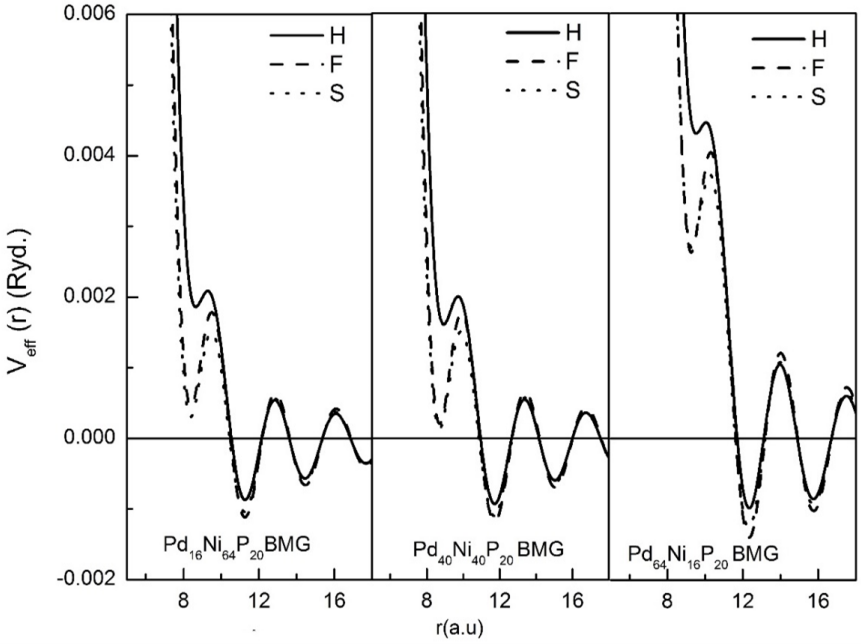

Fig. 1. Pair potential for Pd-Ni-P bulk metallic glasses.

In the present computational study, required input parameters and constants are presented in Table 1. In the present study, our well-tested and modified version of Ashcroft's potential is employed to computing pair potential for the Pd-based bulk metallic glasses. The calculated pair potentials for $Pd_{16}Ni_{64}P_{20}$ BMG, $Pd_{40}Ni_{40}P_{20}$ BMG, and $Pd_{64}Ni_{16}P_{20}$ BMG [6-8] are presented in Fig. 1. It is seen that nature of the pair potential is affected by the $f(q)$. The local field correction

function due to Farid *et al.* [20] influences larger in magnitude compared to Sarkar *et al.* [21]. The first zero for $V_{eff}(r)$ due to F local field correction functions arises at $r_0 \approx 10.55$ (a.u), $r_0 \approx 10.91$ (a.u), and $r_0 \approx 11.61$ (a.u) for $Pd_{16}Ni_{64}P_{20}$ BMG, $Pd_{40}Ni_{40}P_{20}$ BMG and $Pd_{64}Ni_{16}P_{20}$ BMG, respectively.

The phonon dispersion curves for longitudinal and transverse branches are shown in figures 2 to 4, respectively for $Pd_{16}Ni_{64}P_{20}$, $Pd_{40}Ni_{40}P_{20}$ and $Pd_{64}Ni_{16}P_{20}$ BMGs. The PDC for transverse modes achieve maxima at a higher q compared to the longitudinal modes. As the concentration of Pd increases, the collective modes suppressed. This is due to the increasing of the atomic mass of the ternary glass. Also, as the concentration of the Pd increases, the position at which the first maxima occur is shift toward the origin. That is broadening decreases. The influence of various local–field correction functions increase the higher frequencies mode. The local–field correction does not affect appreciably the position of the maxima and minima of longitudinal and transverse modes. Moreover, Chaudhary [8] has computed the phonon dispersion curve using model potential and HB approach but we avoid comparison of PDC to avoid complication in the presentation of graph. From Fig. 3, the results of longitudinal phonon modes in $Pd_{40}Ni_{40}P_{20}$ are closer to a recent experimental study of Hosokawa *et al.* [1]. They have reported phonon modes using the IXS (inelastic X-ray scattering) method [1]. Comparison with the IXS results also supports present data very well. It is seen that the sound velocities in the case of $Pd_{40}Ni_{40}P_{20}$metallic glass is higher than the other two glasses. For the same glass B_T is also higher.

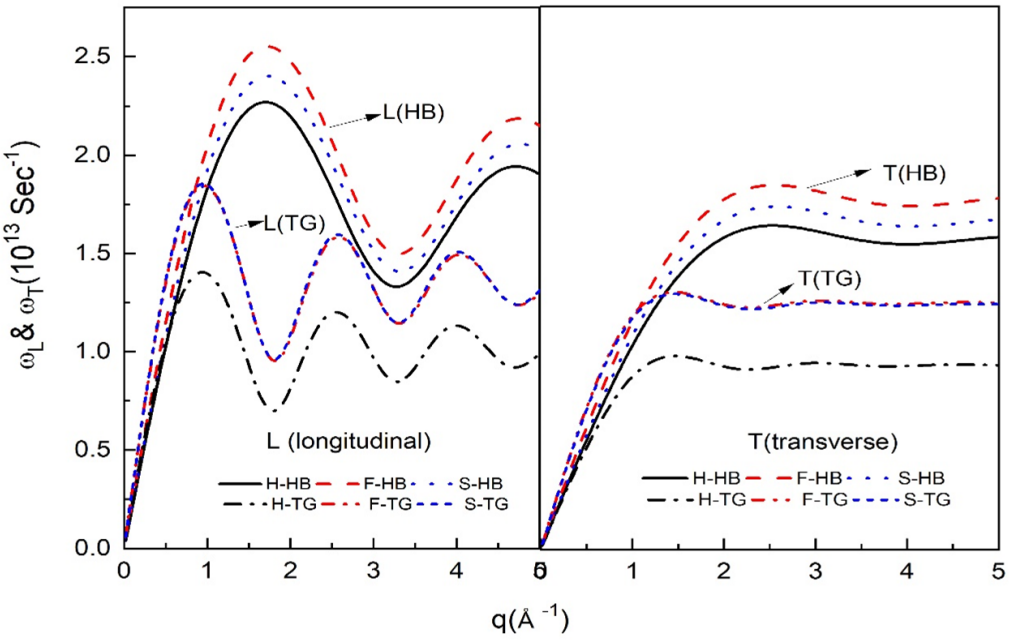

Fig. 2. Phonon dispersion curve of $Pd_{16}Ni_{64}P_{20}$ BMG.

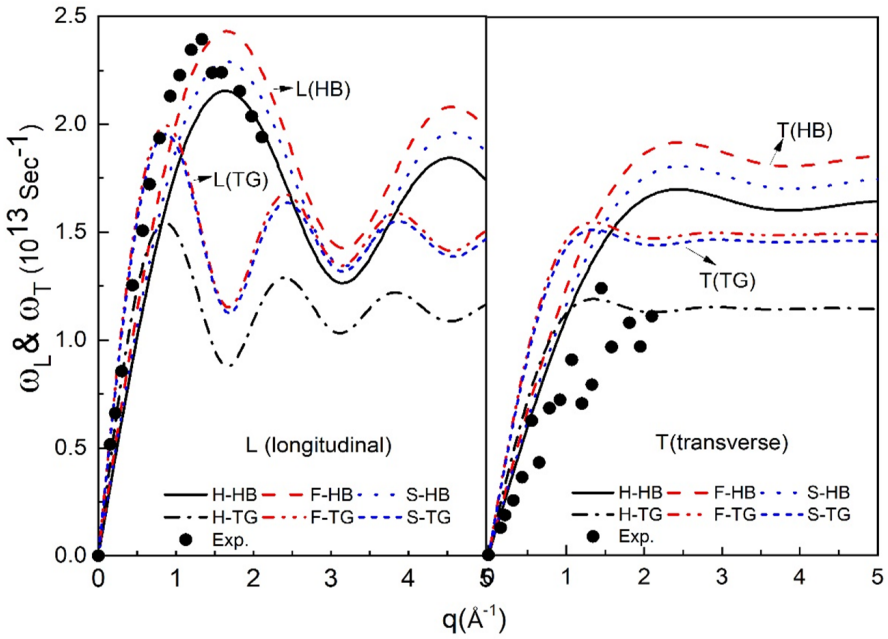

Fig. 3. Phonon dispersive curve of $Pd_{40}Ni_{40}P_{20}$BMG along with experimental data [1].

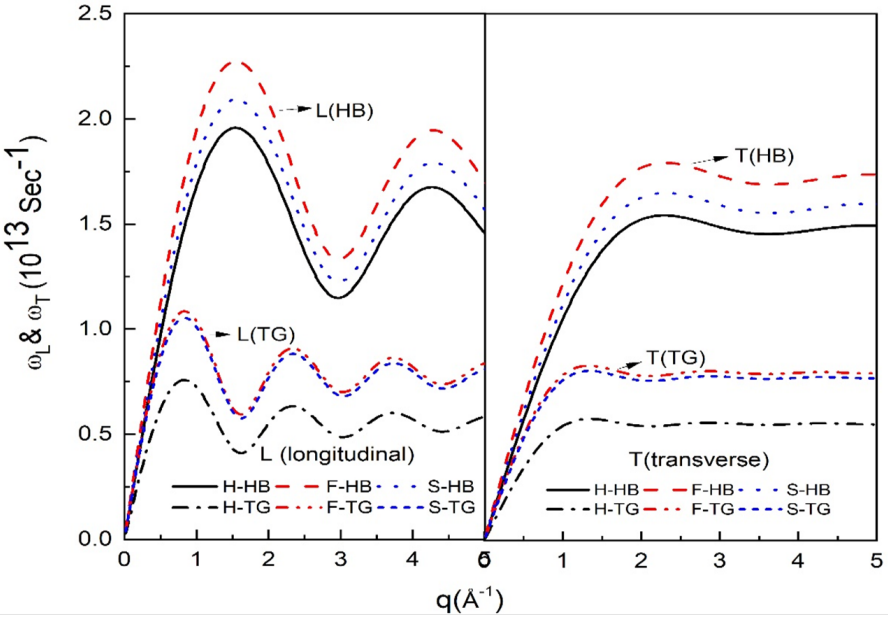

Fig. 4. Phonon dispersive curve of $Pd_{64}Ni_{16}P_{20}$BMG.

The presently computed elastic properties for three metallic glasses and their comparison with the available other theoretically [6, 7] and/or experimentally [1, 7] data are listed in Tables 2 to 4.

Table 2. Elastic and thermodynamics properties of $Pd_{16}Ni_{64}P_{20}$ BMGs.

LFCF→ Properties ↓	**H**		**F**		**S**		**Exp. [6,7]**	**Other [8]**
	HB	**TG**	**HB**	**TG**	**HB**	**TG**		
$\upsilon_L \times 10^5$ **(cm s^{-2})**	4.045	4.334	4.513	5.724	4.226	5.668	5.017	3.87, 3.92, 3.24 3.39, 3.35, 3.29
$\upsilon_T \times 10^5$ **(cm s^{-2})**	2.333	2.234	2.606	3.159	2.439	3.111	2.080	2.24,1.87,1.94 2.27, 1.96, 1.90
B_T **(GPa)**	79.40	106.10	99.01	170.1	56.82	168.2	169.0	204.3,152.8, 163.8 210,167.4,158.0
G (GPa)	47.64	43.65	59.40	87.33	52.09	84.67	37.9	47.1,35.7, 37.8 48.5, 38.6, 36.5
ξ	0.25	0.319	0.25	0.281	0.25	0.284	0.396	0.25
Y (GPa)	127.5	123.8	159.6	240.0	139.9	233.7	105.8	117.9, 88.15, 94.5 121.3, 96.6, 91.2
θ_D**(K)**	337.9	326.2	376.0	459.2	377.4	452.4	–	295.2, 252.5,261.4 299.5, 266.6, 256.8

Table 3. Elastic and thermodynamics properties of $Pd_{40}Ni_{40}P_{20}$ BMGs.

LFCF→ Properties ↓	**H**		**F**		**S**		**Exp. [6,7]**	**Other [8]**
	HB	**TG**	**HB**	**TG**	**HB**	**TG**		
$\upsilon_L \times 10^5$ **(cm s^{-2})**	3.988	5.383	4.473	6.933	4.194	6.757	4.90, 4.87 [1]	2.69, 2.56, 2.83 3.39, 2.82
$\upsilon_T \times 10^5$ **(cm s^{-2})**	2.302	2.445	2.582	3.878	2.421	3.768	1.96, 1.99 [1]	1.55, 1.48, 1.63 1.95, 1.629
B_T **(GPa)**	83.11	163.7	104.5	263.5	91.93	251.3	175.0	105, 95.64, 116.3 167, 116
G (GPa)	49.86	81.55	62.71	141.4	55.14	81.53	36.5	24.4, 22.0, 26.8 38.5, 26.7
ξ	0.25	0.286	0.25	0.272	0.25	0.274	0.40	0.25
Y(GPa)	124.7	209.7	156.8	359.8	137.9	340.3	105.0	61, 55.2, 67.1 96.3, 66.9
θ_D**(K)**	325.56	418.5	365.5	550.2	342.71	534.8	292.0	210.2, 199.8, 220.3264.1, 220.0

Table 4. Elastic and thermodynamics properties of $Pd_{64}Ni_{16}P_{20}$ BMGs.

LFCF→ Properties ↓	**H**		**F**		**S**		**Exp. [6,7]**	**Other** [8]
	HB	**TG**	**HB**	**TG**	**HB**	**TG**		
$\upsilon_L \times 10^5$ (cm s^{-2})	3.850	2.697	4.458	3.863	4.093	3.744	4.560	4.98, 3.38, 4.28 4.3, 2.38, 3.40
$\upsilon_T \times 10^5$ (cm s^{-2})	2.223	1.407	2.574	2.049	2.363	1.979	1.790	2.88, 1.95, 2.47 2.48, 1.37, 1.96
B_T (GPa)	83.04	46.73	111.3	94.04	93.82	88.7	172.0	394.8, 166.5, 267.1 252.2, 128.1, 169.2
G (GPa)	49.8	19.94	66.79	42.30	56.29	39.46	32.8	91.1, 27.5, 58.2 21.9, 22.7
ξ	0.25	0.313	0.25	0.304	0.25	0.306	0.410	0.25
Y (GPa)	124.6	52.37	166.9	110.4	140.7	103.1	93.5	117.9, 96.0, 154.2 145.4,73.83, 97.5
θ_D(K)	306.6	195.4	354.9	284.4	325.9	274.7	256	300.2, 263.6, 333.9 327.9, 231.3, 265.6

IV. CONCLUSION

The present work reports pair potential, phonon dispersion curves and elastic properties for Pd-Ni-P bulk metallic glass using local model potential. The PDCs computed from the HB and TG approaches reproduces all major characteristics of dispersion curves of Pd-Ni-P bulk metallic glasses. The result of longitudinal modes of $Pd_{40}Ni_{40}P_{20}$ are very close to reported data [1]. The model potential with the Farid *et al.* (F) local field correction function generates over all consistent results for PDCs and elastic properties. The obtained elastic properties employing a HB and TG approach with F local field correlation function give good comparison with the experimental results for Pd-Ni-P bulk metallic glasses. The above results also give the confirmation of applicability of the model potential and supports the present method for studying the phonon dynamics and elastic properties of bulk metallic glasses. It is also to note that these results may provide a useful set of data for comparison in future.

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