INFLUENCE OF DIELECTRIC SCREENINGS ON PHONON FREQUENCIES AND ACOUSTIC PROPERTIES OF Pd-BASED BULK METALLIC GLASSES

R.R. Koirenga, P.C. Agarwal, Alpana Gokhroo

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The phonon dispersion curves for bulk metallic glasses (BMGs) Pd40Ni10Cu30P20 and Pd64Ni16P20 are computed for the longitudinal and transverse phonon frequencies using the simple model given by Bhatia and Singh. Different dielectric screening functions are employed for the longitudinal mode. We obtain the values of the force constants \( \beta \) and \( \delta \) calculated from the elastic constants of the material of the respective BMGs for computing the dispersion curves. The computed phonon dispersion curves show appropriate behaviour for both the longitudinal and transverse modes. The transverse sound velocity and the longitudinal sound velocities with various dielectric screenings are calculated in the long wavelength region from the computed dispersion curves for both the BMGs. The first peak position of the static structure factor is predicted from the dispersion curves. The values of sound velocities and the first peak of the static structure factor estimated from the computed dispersion curves show excellent agreement with the experimental values reported in literature for the BMGs under consideration and the results may be used for correlating other properties of the BMGs.

KEYWORDS: Bulk metallic glass, dispersion curves, dielectric screening, elastic properties

The advent of bulk metallic glasses (BMGs) has attracted a lot of interest due to its novel properties and applications in diverse technological areas [1–3]. Pd-based BMGs due to their unique mechanical and thermal properties have shown potential applications as electrode, jewelry and medical materials [4–5]. However, the understanding of phonon dynamics and atomic structure configuration are essential for understanding their mechanical and thermal properties [6–9]. The phonon dynamics of metallic glasses have been studied experimentally [10–11] using neutron scattering. Theoretically computed phonon frequencies have been investigated by many researchers [12–17] for correlating them with mechanical and thermal properties in a variety of metallic glasses. Three main theoretical approaches, namely Hubbard and Beeby [15], Takeno and Goda [16] and that of Bhatia and Singh [8] are widely used for computing phonon frequencies of metallic glasses.

In this paper, the phonon dispersion curves of Pd40Ni10Cu30P20 and Pd64Ni16P20 BMGs computed using the simple model given by Bhatia and Singh [8]. This model assumes a central force which is effective between the nearest neighbours and a volume dependent force. Bhatia and Singh [8] determine the values of force constants \( \delta \) and \( \beta \) using the value of longitudinal and transverse sound velocities along with the calculated value of force constant \( \kappa_e \). However, in the approach adopted by us, we fix the values of force constants \( \delta \) and \( \beta \) used in the computation of dispersion curves by using the value of bulk modulus \( B \) and shear modulus \( G \) of the respective BMGs along with the calculated value of \( \kappa_e \). This method of determining the values of \( \delta \) and \( \beta \) from the elastic moduli of the BMGs for computing phonon frequencies using the simple model is applied for the first time for the Pd40Ni10Cu30P20 and Pd64Ni16P20 BMGs. The dielectric screening due to conduction electrons in the long wavelength region of the phonon frequencies is quite significant. To study its effect on the phonon frequencies, various dielectric screening functions [13] namely, Bhatia and Singh (BS), Hartree (H), Hubbard (HB), Geldart and Vosko (GV), self-consistent screening due to Shaw (SCS) and Overhauser (OH) are employed for the longitudinal mode.

The longitudinal sound velocities \( V_L \) are computed for different dielectric screenings and the transverse sound velocity \( V_T \) is computed from the longitudinal and transverse dispersion curves respectively in the long wavelength region for both the Pd40Ni10Cu30P20 and Pd64Ni16P20 BMGs. The first peak position of the static structure factor \( S(q) \) denoted by \( q_p \) provides key structural information and elastic properties of amorphous materials [7]. The value of \( q_p \) is estimated from the dispersion curves, where it occurs around the first minimum of the longitudinal vibration mode [9].

THEORY

The details of this theory of the simple model employed are given by Bhatia and Singh [8] and others [12–13]. The equations for the longitudinal phonon frequencies \( \omega_L \) and transverse phonon frequencies \( \omega_T \) as given by Bhatia and Singh [8] can be written as

\[
\omega_L^2 = \frac{2N}{\rho a^2} [\beta I_0 + \delta I_2] + \frac{\kappa_e k_F^2 a^4 \sigma_0^2}{\rho [q^2 + \kappa_F^2 \varepsilon(\sigma)]^2},
\]

and
\[ \omega^2 = \frac{2N}{\rho a^2} \left( \beta + \frac{1}{2} \delta \right) I_0 - \frac{1}{2} \delta I_2, \]  

(2)

where \( q \) is the momentum wave vector; \( \beta, \delta \) and \( \kappa_e \) are force constants. \( \beta \) and \( \delta \) are defined in terms of the first and second derivatives of the inter-atomic potential \( W(r) \) at \( r = a \), as

\[ \beta = \frac{\rho a^3}{2M} \left[ \frac{\partial W(r)}{\partial r} \right]_{r=a}, \]  

(3)

\[ \delta = \frac{\rho a^3}{2M} \left[ \frac{\partial^2 W(r)}{\partial r^2} \right]_{r=a}. \]  

(4)

In equation (1), the relevant force constant \( \kappa_e \) due to the conduction electrons based on the Thomas–Fermi model can be written as

\[ \kappa_e = 4\pi e n_i z e^2 / K_{TF}^2, \]  

(5)

where \( e \) is the electron charge, \( n_i \) is the ionic density, \( n_e = n_i z \) is mean electron density and \( z \) is the mean valence of the glassy system; \( K_{TF}^2 = (4k_F/\pi a_0) \) is the Thomas-Fermi screening length with \( a_0 \) as the Bohr radius.

The \( [G(q,r_\circ)]^2 \) in equation (1) is the shape factor to take into account the cancellation effects of kinetic and potential energies inside the core of the ions and is of the form

\[ [G(q,r_\circ)]^2 = \left[ \frac{3(\sin(qr_\circ)-(qr_\circ)\cos(qr_\circ))}{(qr_\circ)^3} \right]^2, \]  

(6)

where \( r_\circ = [3/(4\pi n_i)]^{1/3} \) is the radius of the Wigner-Seitz sphere.

The term \( \epsilon(q) \) in equation (1) is the dielectric screening function. We employ various dielectric screenings [13] namely Bhatia and Singh (BS), Hartree (H), Hubbard (HB), Geldart and Vosko (GV), self-consistent screening due to Shaw (SCS) and Overhauser (OH) in equation (1) to study the effect on phonon frequencies in the long wavelength region.

In equations (1) and (2), \( I_n \) can be written as [8]

\[ I_n = \int_0^\pi \sin \theta \cos^2 \theta \left[ \sin^2 \left( \frac{1}{2} qa \cos \theta \right) \right] d\theta, \]  

(7)

so that with \( x = qa \), \( I_0 \) and \( I_2 \) are respectively,

\[ I_0(x) = 1 - \frac{\sin x}{x}, \]

\[ I_2(x) = \frac{1}{3} - \sin x \left[ \frac{1}{2} - \frac{2 \cos x}{x^2} \right], \]

for the limiting case \( q \to 0 \), equations (1) and (2) give the longitudinal and transverse sound velocities respectively, \( V_L(0) = \omega_L / q \) and \( V_T(0) = \omega_T / q \) as

\[ \rho V_L^2(0) = N \left( \frac{1}{2} \beta + \frac{1}{5} \delta \right) + \kappa_e, \]  

(8)

\[ \rho V_T^2(0) = N \left( \frac{1}{2} \beta + \frac{1}{15} \delta \right). \]  

(9)

In terms of the elastic moduli of the glassy material [8]

\[ C_{11} = \rho V_L^2(0) = B + \frac{4}{3} G, \]  

(10)

\[ C_{44} = \rho V_T^2(0) = G. \]  

(11)

The value of \( \beta \) and \( \delta \) can be determined using equations (8), (9), (10) and (11). The sound velocities for both Pd_{40}Ni_{10}Cu_{30}P_{20} and Pd_{64}Ni_{16}P_{20} BMGs are estimated for the longitudinal mode \( (V_L) \) with different dielectric screenings and transverse mode \( (V_T) \) in the long wavelength region from the respective dispersion curves. The first peak of the static structure factor for both the BMGs is also estimated from the dispersion curves.

**CALCULATIONS**

For the Pd_{40}Ni_{10}Cu_{30}P_{20} BMG, the experimental values of \( B, G \) and \( \rho \) [2] are 172.60×10^9 Nm^{-2}, 35.50×10^9 Nm^{-2} and 9.259×10^3 kgm^{-3} respectively and for the Pd_{64}Ni_{16}P_{20} BMG, the experimental values of \( B, G \) and \( \rho \) [2, 17] are taken as 172.00×10^9 Nm^{-2}, 32.80×10^9 Nm^{-2} and 10.08×10^3 kgm^{-3} respectively. The values of \( n_i \) is calculated using the
relation $\rho = n_t M$ and found to be $7.57 \times 10^{28}$ m$^{-3}$ for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and $7.26 \times 10^{28}$ m$^{-3}$ for Pd$_{64}$Ni$_{16}$P$_{20}$. The two BMGs under consideration are of FCC structure and using the relation $a^3 n_t = \sqrt{2}$, gives $a = 2.65 \times 10^{-10}$ m and $a = 2.69 \times 10^{-10}$ m for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ respectively.

The value of $\kappa_e$ calculated using equation (5) for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ with $z = 1.90$ is $153.50 \times 10^9$ Nm$^{-2}$ and for Pd$_{64}$Ni$_{16}$P$_{20}$ with $z = 2.20$ is $182.75 \times 10^9$ Nm$^{-2}$. Taking $N=12$ for FCC structure for both the BMGs Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$, the values of the respective force constants $\beta$ and $\delta$ for both the BMGs are obtained by substituting the respective values of $B$, $G$ and $\kappa_e$ in equations (8), (9), (10) and (11). Hence all the input parameters for computing phonon dispersion curves for both the BMGs are known and are listed in Table 1.

**Table 1.**

<table>
<thead>
<tr>
<th>Parameters used for computing phonon dispersion curves of Pd$<em>{40}$Ni$</em>{10}$Cu$<em>{30}$P$</em>{20}$ and Pd$<em>{64}$Ni$</em>{16}$P$_{20}$ BMGs.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$n_t$ ($10^{28}$ m$^{-3}$)</td>
</tr>
<tr>
<td>$\kappa_e$ ($10^9$ Nm$^{-2}$)</td>
</tr>
<tr>
<td>$k_F$ ($10^{10}$ m$^{-1}$)</td>
</tr>
<tr>
<td>$r_s$ ($10^{-10}$ m)</td>
</tr>
<tr>
<td>$K_F^2$ ($10^{20}$ m$^{-2}$)</td>
</tr>
<tr>
<td>$\beta$ ($10^9$ Nm$^{-2}$)</td>
</tr>
<tr>
<td>$\delta$ ($10^9$ Nm$^{-2}$)</td>
</tr>
<tr>
<td>$z$</td>
</tr>
</tbody>
</table>

### RESULTS AND DISCUSSION

The phonon dispersion curves computed for the BMGs Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ using the simple model given by Bhatia and Singh [8] are shown in Figure 1a and 1b respectively. The phonon frequency curves for the longitudinal mode employing different dielectric screening functions, namely Bhatia and Singh (BS), Hartree (H), Hubbard (HB), Geldart and Vosko (GV), self-consistent screening due to Shaw (SCS) and Overhauser (OH) for the BMGs Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ are obtained on the basis of equation (1). Similarly, the phonon frequency curves for the transverse mode (T) for the Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ BMGs are obtained on the basis of equation (2) without dielectric screening. The dispersion curves for both the longitudinal mode ($\omega_L$-$q$) as well as the transverse mode ($\omega_T$-$q$) show linear dispersion curves in the long wavelength region and reproduce all the characteristic features as shown in Figure 1a and 1b.

![Figure 1a](image1.png)  ![Figure 1b](image2.png)

**Figure 1.** The transverse (T) phonon frequencies on the basis of equation (2) and longitudinal phonon frequencies due to dielectric screenings viz. BS, H, HB, GV, SCS and OH on the basis of equation (1) for the BMGs (a)Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and (b) Pd$_{64}$Ni$_{16}$P$_{20}$

As seen in Figure 1a and 1b, the dielectric screening functions have significant effect in the long wavelength region of the $\omega_L$-$q$ dispersion curves for both the Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ BMGs. The height of the first peak of the longitudinal vibrations mode depends on the type of dielectric screenings employed for computing the phonon frequencies. From the Figure 1a and 1b, it is evident that the difference in $\omega_L$-$q$ curves for different dielectric screenings
for both the BMGs increases with the wave number $q$ and becomes more prominent at the first maxima and starts decreasing, and the curves converge at the $q$ value corresponding to the first minima of $\omega_{l-q}$ curves.

The position of the first peak of the $\omega_{l-q}$ curves for the Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ BMG are found at $q = 1.3 \times 10^{10}$ m$^{-1}$ for BS, HB, GV, SCS and OH, and at $q = 1.2 \times 10^{10}$ m$^{-1}$ for H. In the case of Pd$_{64}$Ni$_{16}$P$_{20}$ BMG, the position of the first peak for $\omega_{l-q}$ curves are found at $q = 1.2 \times 10^{10}$ m$^{-1}$ for BS, H, HB and OH, and at $q = 1.3 \times 10^{10}$ m$^{-1}$ for GV and SCS. The first minima of the $\omega_{l-q}$ curves for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ are obtained at $q = 2.9 \times 10^{10}$ m$^{-1}$ and $q = 3.0 \times 10^{10}$ m$^{-1}$ respectively, independent of the dielectric screenings employed.

The first peak position of $\omega_{l-q}$ curves for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ are obtained at $q = 1.9 \times 10^{10}$ m$^{-1}$ and $q = 1.7 \times 10^{10}$ m$^{-1}$ respectively. For both the BMGs Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$, the first peak position for $\omega_{l-q}$ curves is at a higher $q$ value than the first peak position of $\omega_{l-q}$ curves for all dielectric screenings. As expected, the $\omega_{l-q}$ dispersion curves for both the BMGs increases and attain peak value with the increase in wave number $q$ and thereafter gets saturated around the first peak with a small variation.

In the long wavelength region ($q \to 0$) of the dispersion curves, the sound velocities of the longitudinal and transverse modes are estimated for both the BMGs. The values of longitudinal velocities ($V_L$) computed from the longitudinal dispersion curves for different dielectric screenings and the transverse velocity ($V_T$) computed from the transverse dispersion curves for both the BMGs Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ are listed in Table 2. The dielectric screenings have significant effect on the longitudinal sound velocity. The experimental values of the longitudinal sound velocity for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ is $4.874 \times 10^5$ cm$^{-1}$ [2] and for Pd$_{64}$Ni$_{16}$P$_{20}$ is $4.560 \times 10^5$ cm$^{-1}$ [2,17]. The values of $V_L$ computed from the dispersion curves for both the BMGs under consideration show closeness to the experimental value for the dielectric screening due to OH. The value of $V_L$ computed from the dispersion curves due to OH screening is $4.839 \times 10^5$ cm$^{-1}$ for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and $4.606 \times 10^5$ cm$^{-1}$ for Pd$_{64}$Ni$_{16}$P$_{20}$. As shown in Table 2, the values of $V_L$ computed for different dielectric screenings for both the BMGs are screening sensitive in the long wavelength region.

### Table 2

<table>
<thead>
<tr>
<th>Dielectric screenings</th>
<th>Pd$<em>{40}$Ni$</em>{10}$Cu$<em>{30}$P$</em>{20}$</th>
<th>Pd$<em>{64}$Ni$</em>{16}$P$_{20}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$V_L (10^5$ cm$^{-1}$)</td>
<td>$V_T (10^5$ cm$^{-1}$)</td>
</tr>
<tr>
<td>BS</td>
<td>5.358</td>
<td>1.827</td>
</tr>
<tr>
<td>HB</td>
<td>4.949</td>
<td>4.722</td>
</tr>
<tr>
<td>SCS</td>
<td>4.232</td>
<td>3.931</td>
</tr>
</tbody>
</table>

The transverse sound velocity ($V_T$) computed from the slope of the dispersion curves in the elastic region for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ is $1.827 \times 10^5$ cm$^{-1}$ and for Pd$_{64}$Ni$_{16}$P$_{20}$ is $1.735 \times 10^5$ cm$^{-1}$. The experimental values of transverse sound velocities reported for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ are $1.959 \times 10^5$ cm$^{-1}$ [2] and $1.790 \times 10^5$ cm$^{-1}$ [2,17] respectively. Thus, the computed transverse sound velocities are very close to the experimental values reported for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$.

From the $\omega_{l-q}$ curves of the BMGs under consideration, we estimate the first peak position ($q_p$) of the static structure factor $S(q)$. The first minimum of $\omega_{l-q}$ curves occurs around the same value of the wave number $q$ where the first peak $q_p$ of the static structure factor $S(q)$ occurs [9]. The position of the first minimum estimated from the $\omega_{l-q}$ curves for the BMGs Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$ occur at $q = 2.9 \times 10^{10}$ m$^{-1}$ and $q = 3.0 \times 10^{10}$ m$^{-1}$ respectively, independent of the dielectric screenings. The computed values of $q_p$ for both the BMGs are given in Table 3. The experimental reported value of the first peak position $q_p$ of the static structure factor for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ is $q = 2.9 \times 10^{10}$ m$^{-1}$ [7] (Table 3). However, no experimental data for the static structure factor of Pd$_{64}$Ni$_{16}$P$_{20}$ BMG is available, we estimate from the theoretical phonon dispersion curves to be at $q = 3.0 \times 10^{10}$ m$^{-1}$.

### Table 3

<table>
<thead>
<tr>
<th>BMGs</th>
<th>$q_p (10^{10}$ m$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pd$<em>{40}$Ni$</em>{10}$Cu$<em>{30}$P$</em>{20}$</td>
<td>2.9, 2.9 [7]</td>
</tr>
<tr>
<td>Pd$<em>{64}$Ni$</em>{16}$P$_{20}$</td>
<td>3.0</td>
</tr>
</tbody>
</table>

The computed values of $q_p$ for both the BMGs are slightly less than $2k_F$, where $k_F$ is calculated using the relation, $k_F = (3\pi^2n_c)^{1/3}$. The calculated values of $k_F$ are $1.62 \times 10^{10}$ m$^{-1}$ for Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and $1.68 \times 10^{10}$ m$^{-1}$ for Pd$_{64}$Ni$_{16}$P$_{20}$ (Table 1). The ratio of $2k_F/q_p$ is 1.12 for both the BMGs Pd$_{40}$Ni$_{10}$Cu$_{30}$P$_{20}$ and Pd$_{64}$Ni$_{16}$P$_{20}$. This is in agreement with the
stability of metallic glasses [18]. Since the peak position of the structure factor provides key structural information in understanding atomic network for amorphous materials, it is used for correlating with elastic properties of BMGs [7]. From the results obtained from the dispersion curves, we can infer that the value of \( q_p \) is not affected by the dielectric screening functions, though the dielectric screenings have a significant effect on the values of the longitudinal sound velocities for the BMGs.

CONCLUSION

We have computed the phonon dispersion curves for Pd\(_{60}\)Ni\(_{10}\)Cu\(_{30}\)P\(_{20}\) and Pd\(_{64}\)Ni\(_{16}\)P\(_{20}\) BMGs employing various dielectric screenings using the simple model by Bhatia and Singh. The force constants \( \delta \) and \( \beta \) used in the computation of the phonon frequencies are determined using the experimental values of bulk modulus (B) and shear modulus (G) along with the calculated value of force constant \( k_c \) of the BMGs under consideration for the first time. The computed dispersion curves reproduce the main characteristic of phonon frequencies of transverse and longitudinal modes. The values of the transverse and longitudinal velocities estimated from the dispersion curves show excellent agreement with the available value reported in literature for Pd\(_{60}\)Ni\(_{10}\)Cu\(_{30}\)P\(_{20}\). Since the experimental data for phonon frequencies are rare and the limitation of the experimental values reported for both the BMGs. The position of the first peak of the static structure factor for both the BMGs are estimated from the dispersion curves and show excellent agreement with the available value reported in literature for Pd\(_{60}\)Ni\(_{10}\)Cu\(_{30}\)P\(_{20}\). Since the experimental data for phonon frequencies are rare and the limitation of the experimental techniques for describing the micro-structure of metallic glasses, the approach presented in this paper using the Bhatia and Singh model can be employed for computing phonon frequencies. It is expected that appropriate theoretical computation of phonon dispersion curves will give insight in understanding the structural information and elastic properties of metallic glasses.

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поздовжні швидкості звуку з різним діелектричним екрануванням обчислюються в області довжини довжини хвилі з обчислених кривих дисперсії для обох ОМС. Положення першого пика коефіцієнта статичної структури передбачено з дисперсійних кривих. Значення швидкостей звуку та перший пік коефіцієнта статичної структури, розраховані на основі обчислених дисперсійних кривих, показують чудову узгодженість з експериментальними значеннями, що наявні в літературі для розглянутих ОМС, і резултати можуть бути використані для кореляції інших властивостей ОМС.

КЛЮЧОВІ СЛОВА: об’ємне металеве скло, дисперсійні криві, діелектричний екран, еластичні властивості

ВЛИЯНИЕ ДИЭЛЕКТРИЧЕСКОЙ ЭКРАНИРОВКИ НА ФОНОННЫЕ ЧАСТОТЫ И АКУСТИЧЕСКИЕ СВОЙСТВА МЕТАЛЛИЧЕСКИХ СТЕКОЛ НА ОСНОВЕ Pd

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Кривые дисперсии фононов для объемных металлических стекол (ОМС) Pd$40Ni10Cu30P20 и Pd$64Ni16P20 исчисляются для продольной и поперечной частот фононов с помощью простой модели, предоставленной Бхатия и Сингхом. Для продольного режима используются различные функции диэлектрического экранирования. Мы получили значения силовых констант силы β и δ, рассчитанных по упругим константам материала соответствующих ОМС для вычисления кривых дисперсии. Вычисленные кривые дисперсии фононов демонстрируют надлежащее поведение как для продольной, так и для поперечной мод. Поперечная скорость звука и продольные скорости звука с разным диэлектрическим экранированием исчисляются в области длины длины волны из вычисленных кривых дисперсии для обеих ОМС. Положение первого пика коэффициента статической структуры предсказано из дисперсионных кривых. Значения скоростей звука и первый пик коэффициента статической структуры, рассчитанные на основе вычисленных кривых дисперсии, показывают хорошее согласие с экспериментальными значениями, имеющимися в литературе для рассматриваемых ОМС, и результаты могут быть использованы для корреляции других свойств ОМС.

КЛЮЧЕВЫЕ СЛОВА: объемное металлическое стекло, дисперсионные кривые, диэлектрический экран, эластичные свойства