Study of phonon modes and elastic properties of \( \text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) and \( \text{Gd}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) rare-earth bulk metallic glasses

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Abstract. A phonon modes and elastic properties of two different rare-earth based bulk metallic glasses \( \text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) and \( \text{Gd}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) are computed using Hubbard-Beeby approach and our well established model potential. The local field correlation functions due to Hartree (H), Taylor (T), Ichimaru and Utsumi (IU), Farid et al (F) and Sarkar Sen et al (S) are employed to investigate the influence of the screening effects on the vibrational dynamics of \( \text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) and \( \text{Gd}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) bulk metallic glasses. The results for bulk modulus \( B_T \), modulus of rigidity \( G \), Poisson’s ratio \( \xi \), Young’s modulus \( Y \), Debye temperature \( \Theta_D \), propagation velocity of elastic waves and dispersion curves are reported. The computed elastic properties are found to be in good agreement with experimental and other available data.

1. Introduction
Recently formation of rare- earth based bulk metallic glassy (rare earth-Al-Co-Y) alloys are distinguished itself from other metallic glasses due to their better glasses forming ability. Moreover, rare-earth based bulk metallic glasses have attracted more attention for their unique physical properties. Such as mechanical properties, magnetic properties, elastic properties, thermo plastic behaviour and bond properties of material are one of the key issues for both scientific significance and practical application in condensed matter physics [1-4].

In regards of these Wang [4] has reported the development of series of the rare-earth based bulk metallic glasses with desirable properties based on the correlation. The elastic properties of metallic glass can be roughly predicted to guide the selection of alloying elements for developing rare-earth base bulk metallic glass (BMG) with higher glass forming ability (GFA). In the present paper, focus is given on the \( \text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) and \( \text{Gd}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) rare-earth bulk metallic glasses [4] and the computation is carried out for phonon dispersion curve (PDC), bulk modulus \( B_T \), Poisson’s ratio \( \xi \), modulus of rigidity \( G \), Young’s modulus \( Y \) and Debye temperature \( \Theta_D \) [5-7]. Our well recognized bare-ion model potential of the following form is to describe bare ion interaction [8].
\[ V_b(q) = -\frac{4\pi Z e^2}{\Omega_0 q^2} \left[ \cos(qr) - \frac{\exp(-1)q_r}{1 + q_r^2 r_c^2} \{ \sin(qr) + q_r \cos(qr) \} \right] \]  

Here \( Z, \Omega, q, e \) and \( r_c \) are the valency, atomic volume, wave vector, charge of electron and the parameter of the potential respectively. The five exchange and correlation function due to Hartree (H) (without exchange and correlation effect) \([9]\), Taylor (T) \([10]\), Ichimaru and Utsumi (IU) \([11]\), Farid et al (F) \([12]\) and Sarkar Sen et al (S) \([13]\) are employed for the investigation of relative effect of local field correction function on PDC and elastic properties of \( \text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) and \( \text{Gd}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20} \) Bulk metallic glasses.

2. Theory

The effective interaction pair potential for the bulk metallic glass as a one metallic fluid, i.e, the concepts of effective atom \([6, 7]\), can be written as \([6, 7]\)

\[ V_{\text{eff}}(r) = \left( \frac{Z_{\text{eff}}^2 e^2}{r} \right) + \frac{\Omega_{0\text{eff}}}{\pi} \int F_{\text{eff}}(q) \left[ \frac{\sin(qr)}{qr} \right] q^2 dq \]  

Here \( Z_{\text{eff}} \) and \( \Omega_{0\text{eff}} \) are the effective valence and atomic volume of present system respectively. The energy wave number characteristics appearing in the equation (2) is written as \([6, 7]\)

\[ F_{\text{eff}}(q) = \left( -\frac{\Omega_{0\text{eff}}}{16 \pi} \right) \left[ V_{\text{b eff}}(q) \right] \left[ \frac{\varepsilon_{\text{eff}}^H(q) - 1}{1 + \varepsilon_{\text{eff}}^H(q) - 1} \right] \left[ 1 - f_{\text{eff}}(q) \right] \]  

Here ,\( V_{\text{b eff}}(q) \) is effective bare ion potential it is given in equation (1), \( \varepsilon_{\text{eff}}^H(q) \) is the Hartree dielectric response function and \( f_{\text{eff}}(q) \) is the local field correction functions to introduce the exchange and correction effects. A quality which is equally important as the pair potential while studying a disorder system is pair correlation functions \( g(r) \), which is computed theoretically from the effective pair potential.

In the Hubbard and Beeby \([5]\) approach, the longitudinal and transverse phonon frequencies are computed using \([5-7]\);

\[ \omega^2_L(q) = \omega^2_E \left[ 1 - \frac{3 \sin(q\sigma)}{q\sigma} - \frac{6 \cos(q\sigma)}{(q\sigma)^2} + \frac{6 \sin(q\sigma)}{(q\sigma)^3} \right] \]  

\[ \omega^2_T(q) = \omega^2_E \left[ 1 + \frac{3 \cos(q\sigma)}{(q\sigma)^2} - \frac{6 \sin(q\sigma)}{(q\sigma)^3} \right] \]  

Here, \( \omega_E \) represents the maximum phonon frequency and is given as

\[ \omega_E = \frac{4\pi n_{\text{eff}}}{3 M_{\text{eff}}} \int_0^\infty g(r)r^2 V_{\text{eff}}(r)dr \]
\[ V_{\text{eff}}(r) = \frac{4Z^2}{r^3} + \frac{\Omega_0}{\pi^2} \int_0^\infty F(q)q^2 \left[ \frac{2\sin(qr)}{qr^3} - \frac{2\cos(qr)}{r^2} - \frac{q\sin(qr)}{r} \right] dq , \] (7)

and

\[ g(r) = \exp\left[ -\frac{V_{\text{eff}}(r)}{k_BT} \right] - 1 \] (8)

Here, \( \rho, M, g(r), \Omega_0, \) and \( f(q) \) be the number density, atomic mass, pair correlation function, atomic volume and energy wave number characteristic, respectively.

In the long-wavelength limit, the phonon dispersion curve shows an elastic behaviour. Hence, the longitudinal \( \nu_l \) and transverse \( \nu_t \) sound velocities are also calculated by

\[ \nu_l = \omega_E \left( \frac{3s}{10} \right)^{1/2} \quad \text{and} \quad \nu_t = \omega_E \left( \frac{s}{10} \right)^{1/2} \]

Various elastic properties are then determined by the longitudinal and transverse phonon frequencies.

The bulk modulus \( B_T \), Poisson’s ratio \( \xi \), modulus of rigidity \( G \), Young’s modulus \( Y \) and the Debye temperature \( \theta_D \) are calculated using the expression below\[6, 7,\]

\[ B_T = \rho \left( \nu_l^2 - \frac{4}{3} \nu_t^2 \right) \] (10)

\[ G = \rho \nu_t^2 \] (11)

\[ \xi = \frac{1 - 2(\nu_l^2/\nu_t^2)}{2 - 2(\nu_l^2/\nu_t^2)} \] (12)

\[ Y = 2G(\xi + 1) \] (13)

and

\[ \theta_D = \frac{\hbar}{k_B} \left[ \frac{9\rho}{4\pi} \left( \frac{1}{\nu_l^3} + \frac{2}{\nu_t^3} \right)^{1/3} \right] \] (14)

Where, \( \rho \) is the isotropic density of the solid, ‘\( h \)’ is plank constant and \( k_B \) is the Boltzmann constant.
3. Results and Discussions

| Parameters | $\text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ BMG | $\text{Gd}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ BMG |
|------------|---------------------------------|---------------------------------|
| $Z_{\text{eff}}$ | 2.80 | 2.80 |
| $\Omega_{\text{eff}}$ (au)$^3$ | 146.98 | 166.61 |
| $r_{\text{min}}^{\text{eff}}$ (au) | 1.1846 | 1.2350 |
| $M_{\text{eff}}$ (amu) | 52.228 | 92.652 |

The input parameters and constants required for the present study are shown in Table 1. Our well established model potential [8] is used along with five different local field correction functions for the first time to generate pair potential for the $\text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ and $\text{Gd}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ rare-earth bulk metallic glasses system. From figure 1 and figure 2 it is observed that position of the first minima is affected by the type of screening functions. The maximum depth in the pair potential in the present study is obtained due to S screening function. It is also noticed that the first zero for $V(r = r_0)$ due to five local field correction functions occurs at $r_0 = 12.52$ Å and $r_0 = 14.84$ Å for the $\text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ and $\text{Gd}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ rare-earth bulk metallic glasses, respectively. The oscillatory nature is also seen even at large $r$-region.

![Figure 1. Effective pair potential of $\text{Sc}_{36}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ BMG.](image)
**Figure 2.** Effective pair potential of $\text{Gd}_{30}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ BMG.

![Effective pair potential of $\text{Gd}_{30}\text{Al}_{24}\text{Co}_{20}\text{Y}_{20}$ BMG.](image)

**Figure 3.** Longitudinal and transverses phonon modes of $\text{Sc}_{36}\text{Al}_{34}\text{Co}_{20}\text{Y}_{20}$ BMG.

![Longitudinal and transverses phonon modes of $\text{Sc}_{36}\text{Al}_{34}\text{Co}_{20}\text{Y}_{20}$ BMG.](image)
The computed results of the PDC generated using HB scheme along with five different screening functions are shown in figure 3 and figure 4 for the Sc$_{36}$Al$_{24}$Co$_{20}$Y$_{20}$ and Gd$_{36}$Al$_{24}$Co$_{20}$Y$_{20}$ rare-earth bulk metallic glasses, respectively. From figures 3-4, it is observed that the inclusion of local field correction function raises the phonon frequencies in both longitudinal as well as transverse branches. The first minimum in the longitudinal branch of Sc$_{36}$Al$_{24}$Co$_{20}$Y$_{20}$ BMG falls at $q \approx 1.41 - 1.42$ Å$^{-1}$ and similarly the first minimum in the longitudinal branch of Gd$_{36}$Al$_{24}$Co$_{20}$Y$_{20}$ BMG fall at $q \approx 1.47 - 1.48$ Å$^{-1}$. In an absence of experimental data for structure factors, we can offer reverse comment that the structure factor $S(q)$ will show it’s at these $q$s. It is also noticed that the related magnitude of first peak of PDC increasers but the position of first peak is not affected by different screening functions. Phonons of transverse branch undergo large thermal modulation due to anharmonicity of lattice vibrations in this branch. In the long wave length limit, the dispersion curves are linear and confirming characteristics of elastic wave.

### Table 2. Elastic properties of Sc$_{36}$Al$_{24}$Co$_{20}$Y$_{20}$ BMG.

| Properties | H [9]   | T [10]  | IU [11] | F [12]  | S [13]  | Exp. [4] |
|------------|---------|---------|---------|---------|---------|---------|
| $v_L \times 10^7$ (cm s$^{-2}$) | 4.2442  | 4.8069  | 4.8155  | 4.8406  | 4.4569  | --      |
| $v_T \times 10^5$ (cm s$^{-2}$) | 2.4504  | 2.7753  | 2.7802  | 2.7947  | 2.5732  | --      |
| $B_T$ (GPa) | 43.982  | 56.418  | 56.620  | 57.212  | 48.502  | 77.5    |
| $G$ (GPa) | 26.389  | 33.851  | 34.327  | 34.327  | 29.101  | 32.3    |
| $\xi$ | 0.25    | 0.25    | 0.25    | 0.25    | 0.25    | 0.31    |
| $Y$ (GPa) | 65.973  | 84.626  | 84.930  | 85.818  | 72.753  | 85.2    |
| $\theta_D$ (K) | 290.10  | 328.56  | 329.15  | 330.87  | 304.64  | --      |
Presently computed elastic properties for Sc\(_{36}\)Al\(_{24}\)Co\(_{20}\)Y\(_{20}\) and Gd\(_{36}\)Al\(_{24}\)Co\(_{20}\)Y\(_{20}\) rare-earth bulk metallic glasses are listed in table 2 and table 3, respectively. From these tables, one can see that the values are obtained due to T, IU and F screening functions are very close to one another as compared to the H and S screening functions. The experimental only data for bulk modulus ‘\(B_T\)’, modulus of rigidity ‘\(G\)’, Poisson’s ration ‘\(\xi\)’ and Young modulus ‘\(Y\)’ are available. The comparison shows that presently computed results are lower for bulk modulus ‘\(B_T\)’ in both the bulk metallic glasses. The excellent is achieved for modulus of rigidity ‘\(G\)’ and Young modulus ‘\(Y\)’. Since the unavailability of experimental or other theoretical results of collective excitations for these bulk metallic glasses, we are unable to compare the longitudinal and transverse phonon frequencies and Debye temperature of these bulk metallic glasses.

We have also computed maximum and minimum percentile deviation for the elastic properties of bulk modulus, modulus of rigidity and Young modulus with the available experimental data from table 2-3, respectively. In the case of bulk modulus, the computed maximum percentile deviation with respect to the available experimental data is found for H function and the values are 43.29% and 22.56% for Sc metallic glasses, respectively and minimum deviation is found for H function and the values are 18.30% and 13.25% for Sc metallic glasses, respectively. Similarly, for Young’s modulus, the computed maximum percentile deviation is found for H function and the values are 6.27% and 2.52% for Sc metallic glasses, respectively and minimum deviation is found for IU and S functions, the values are 6.27% and 2.52% for Sc metallic glasses, respectively. Minimum deviation is found for F and S functions, the values are 0.45% and 0.25% for Sc metallic glasses, respectively. Moreover, we have also calculated the relative influence of various local field correlation functions with respect to the static H-dielectric function. From table 2, the percentile influence for sound velocity for T, IU, F and S are resulted as 13.25%, 13.46%, 14.05% and 5.01% respectively. The percentile influence for bulk metallic glasses, modulus of rigidity, Young’s modulus and Debye temperature for T, IU, F and S screening functions are computed as 28.27%, 28.73%, 30.08% and 13.25% respectively. With respect to the highest influence of H- screening function is observed for F local field correlation function.

From table 3, we have calculated the percentile influence for sound velocity for T, IU, f and S screening functions are resulted as 14.96%, 15.08%, 15.78% and 6.12% respectively. While percentile influence for bulk metallic glasses, modulus of rigidity, Young modulus and Debye temperature for T, IU, F and S screening functions are computed as 32.18%, 32.43%, 34.04% and 12.61% respectively. It is also observed that the F screening function gives the highest influence over H-screening function then other. However, the present findings are significant when comparison is
carried out with the results of elastic constants, and it is found in line and supports the pseudopotential used in the present investigations. From this calculation it is observed that the presently computed data serve as guideline for further research in this direction.

4. Conclusion
We conclude here that the PDC generated from the HB approach reproduces satisfactorily general characteristics of dispersion curves for Sc$_{36}$Al$_{24}$Co$_{20}$Y$_{20}$ and Gd$_{36}$Al$_{24}$Co$_{20}$Y$_{20}$ bulk metallic glasses. The rare-earth bulk metallic glasses have not been investigated theoretically previously adopting model potential formalism and HB approach. The present local model potential depends on effective core radius which is used here to describe the electron-ion interaction. It is obvious that the present results are generated without any fitting procedure. This also confirms the applicability of the model potential in the aforesaid properties and supports the present approach.

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