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Phonon Modes and Elastic Properties of RE55Al25Co20 Bulk Metallic Glasses

P. H. Suthar

Department of Physics, C U Shah Science College, Ashram Road, Ahmedabad, Gujarat, India

ABSTRACT

The present paper deals with the theoretical study of phonon modes and elastic properties of RE55Al25Co20 (RE (Rare Earth) =Y, La, Ce, Pr, Nd, Sm, Gd, Tb, Dy, Ho, Er, Tm, Lu) bulk metallic glasses. The Hubbard-Beeby approach combine with Jani et al. local model potential has been utilized to compute the collective modes for present glasses. Three different local field correlation functions of Hartree (H), Taylor (T) and Farid et al (F) are employed to find the influence of the screening effects on the collective modes of RE55Al25Co20 bulk metallic glasses. The calculated phonon dispersion curves show all broad features of the collective excitation. It observed that out of three local field correction function, Taylor and Farid et al screening functions give better agreement with experimental values compared to other screening functions. Overall, the present results of elastic properties are found to be good agreement with experimental results.

KEYWORDS: *Bulk Metallic Glass, Pseudo potential, Local field correction function, Collective modes, elastic properties*

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INTRODUCTION

The bulk metallic glass (BMG) alloys have been considered as a special interest in the material science research over the last six decades. From the literature survey, bulk metallic glasses show unique structural features and outstanding mechanical, many novels, applying chemical and physical properties [1-9] because of glassy states, is associated widely with daily life, industry, materials preparation, organism preservation and a lot of natural phenomena [1-13].

Here, it has focused on rare earth base bulk metallic glasses (RE-Al-Co, {RE (rare earth) = Y, La, Ce, PR, Nd, Sm Gd, Tb, Dy, Ho, Er, Tm, Lu (lanthanide series)}) [3,4]. These glasses have distinguished itself from other metallic glasses due to their better glasses forming ability. Furthermore, rare-earth based bulk metallic glasses have concerned more attention for their unique physical properties. Such as mechanical properties, magnetic properties, elastic properties, thermodynamics, thermoplastic behaviour and bond properties of materials are one of the main topics for both scientific significance and practical application in condensed matter physics, materials science and engineering [1-13].

In regards of these Wang et al [3, 4] have reported the development of a series of the rare-earth (RE-Al-Cu) 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 a rare-earth base bulk metallic glass (RE-BMG) with higher glass forming ability (GFA). In this article, It is attention on the computation is carried out for phonon dispersion curve (PDC) and elastic properties likewise longitudinal sound velocity 'V_L', transverse sound velocity 'V_T', bulk modulus B_T, Poisson's ratio ν, modulus of rigidity G, Young's modulus Y and Debye temperature Θ_D with the help of Hubbard Beeby [11] approach and model potential given by Jani et al [12-13] along with three different screening functions due to Hartree (H) [14], Taylor (T) [15] and Farid et al (F) [16] for the $RE_{55}Al_{25}Co_{20}$ rare-earth bulk metallic glasses [3,4].

COMPUTATIONAL METHOD

Hubbard and Beeby (HB) [11], Takeno and Goda (TG) [17, 18] and Bhatia and Singh (BS) are main theoretical approaches used to calculate the phonon dispersion curve (PDC). One is the phenomenological theory of HB [11] in the random phase approximation, TG is the quasi-crystalline approximation technique with interatomic pair potential. And the third is by evaluation of force constants as was done by BS [19].

Out of this three theoretical approaches, The HB theoretical model has been utilized here to generate the phonon dispersion curves (PDC) of bulk metallic glasses of specific concentration ($RE_{55}Al_{25}Co_{20}$) in the present computation.

A. Model potential and Pair Potential

The selection of model potential is an important aspect as it will describe the motion of valance electrons in a metal. For the present study, we have used single parametric local model pseudopotential of the following form in the q-space. [10, 12, 13].

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

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.

The effective interaction pair potential for the bulk metallic glass as a one metallic fluid, i.e, the concepts of effective atom [10], can be written as [10, 13]

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

Here Z_{eff} and Ω_{0eff} are the effective valence and atomic volume of present system respectively.

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.

The energy wave number characteristics appearing in the equation (2) are written as [10-12]

$$F_{eff}(q) = \left(\frac{-\Omega_{0eff}}{16\pi}\right)\left|V_b^{eff}(q)\right|^2 \frac{\left[\varepsilon_H^{eff}(q) - 1\right]}{\left\{1 + \left[\varepsilon_H^{eff}(q) - 1\right]\left[1 - f_{eff}(q)\right]\right\}} \quad (3)$$

Here, $V_b^{eff}(q)$ is effective bare ion potential it is given in equation (1), $\varepsilon_H^{eff}(q)$ is the Hartree dielectric response function [12] and $f_{eff}(q)$ is the local field correction functions to introduce the exchange and correction effects. The three exchange and correlation function due to Hartree (H) (without exchange and correlation effect) [15], Taylor (T) [12], and Farid et al (F) [13] are employed for the investigation of the relative effect of the local field correction function on PDC and elastic properties of $RE_{55}Al_{25}Co_{20}$ Bulk metallic glasses.

B. Phonon Dispersion Curve and Elastic Constants

The In the Hubbard and Beeby [13] approach, the longitudinal and transverse phonon frequencies are computed using [10, 11, 13];

$$\omega_L^2(q) = \omega_E^2\left[1 - \frac{3\sin(q\sigma)}{q\sigma} - \frac{6\cos(q\sigma)}{(q\sigma)^2} + \frac{6\sin(q\sigma)}{(q\sigma)^3}\right] \quad (4)$$

$$\omega_T^2(q) = \omega_E^2\left[1 + \frac{3\cos(q\sigma)}{(q\sigma)^2} - \frac{6\sin(q\sigma)}{(q\sigma)^3}\right] \quad (5)$$

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

$$\omega_E = \frac{4\pi n_{eff}}{3M_{eff}}\int_0^\infty g(r) r^2 V_{eff}''(r) dr \quad (6)$$

With

$$V_{eff}''(r) = \frac{4Z_{eff}^2}{r^3} + \frac{\Omega_{0eff}}{\pi^2}\int_0^\infty F_{eff}(q) q^2 \left[\frac{2\sin(qr)}{qr^3} - \frac{2\cos(qr)}{r^2} - \frac{qsin(qr)}{r}\right] dq \quad (7)$$

and

$$g(r) = \exp\left[\left(\frac{-V_{eff}''(r)}{k_B T}\right) - 1\right] \quad (8)$$

Here, ρ, M_{eff}, $g(r)$, Ω_{0eff}, and $F_{eff}(q)$ 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 ν_l and transverse ν_t sound velocities are also calculated by [10,11]

$$\nu_l = \omega_E\left(\frac{3\xi}{10}\right)^{1/2} \text{ and } \nu_t = \omega_E\left(\frac{\xi}{10}\right)^{1/2} \quad (9)$$

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

The bulk modulus B_T, Poisson's ratio ξ, modulus of rigidity G, Young's modulus Y and the Debye temperature θ_D are calculated using the expression below [10,11]

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

$$G = \rho\nu_t^2 \quad (11)$$

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

$$Y = 2G(\xi + 1) \quad (13)$$

and

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

Where, ρ is the isotropic density of the solid, 'h' is plank constant and k_B is the Boltzmann constant.

RESULTS AND DISCUSSION

TABLE I.: Input parameters and constants for $RE_{55}Al_{25}Co_{20}$ bulk metallic glasses

Parameters → BMG ↓	Z_{eff}	Ω_{0eff} [au]³	R_{ceff} [au]	M_{eff} [amu]
$Y_{55}Al_{25}Cu_{20}$	2.085	161.29	1.620	54.09
$La_{55}Al_{25}Cu_{20}$		183.28	1.607	94.93
$Ce_{55}Al_{25}Cu_{20}$		184.66	1.697	95.59
$Pr_{55}Al_{25}Cu_{20}$		168.79	1.712	96.03
$Nd_{55}Al_{25}Cu_{20}$		166.50	1.727	97.86
$Sm_{55}Al_{25}Cu_{20}$		172.23	1.730	101.2
$Gd_{55}Al_{25}Cu_{20}$		155.76	1.675	102. 1
$Tb_{55}Al_{25}Cu_{20}$		158.47	1.694	101.9
$Dy_{55}Al_{25}Cu_{20}$		159.89	1.868	107.9
$Ho_{55}Al_{25}Cu_{20}$		155.47	1.694	109.2
$Er_{55}Al_{25}Cu_{20}$		151.78	1.730	109.2
$Tm_{55}Al_{25}Cu_{20}$		150.88	1.618	110.5
$Lu_{55}Al_{25}Cu_{20}$		147.86	1.651	114.7

All the calculations have been performed for the $RE_{55}Al_{25}Co_{20}$ bulk metallic glasses. The input parameters and constants used in the present investigation of the phonon dispersion curve and elastic properties are tabulated in Table 1. Jani et al [14] model potential is used along with three different local field correction functions for the generate pair potential for the $RE_{55}Al_{25}Co_{20}$ rare-earth bulk metallic glass system. From Fig. 1, it is observed that the 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 F screening function for $Ce_{55}Al_{25}Co_{20}$ BMG compared to other rare earth bulk metallic glasses. It is also noticed that the first zero for $V(r = r_0)$ due to Hatree (H) $r_0 = 13.76au \sim 15.21au$, for Taylor (T) [16] $r_0 = 13.69au \sim 15.08\,au$ and for Farid et (F) [17] $r_0 = 13.71au \sim 15.10\,au$ are occurring for local field correction functions for $RE_{55}Al_{25}Co_{20}$ rare-earth bulk metallic glasses. The oscillatory nature is also seen even at large *r*-region.

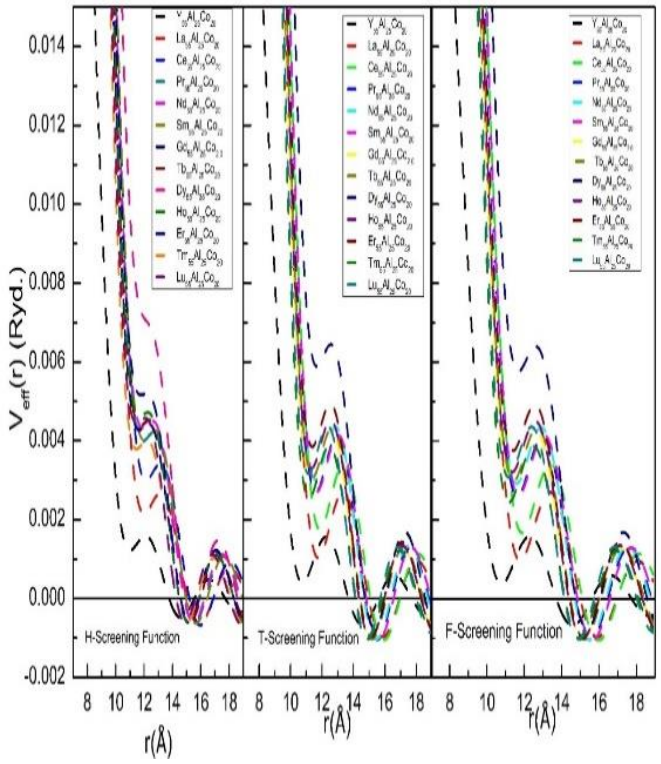

Fig.1 Screening dependence effective pair potential of $RE_{55}Al_{25}Co_{20}$ BMG

The computed results of the longitudinal phonon dispersion curve (ω_L) and transverse phonon dispersion curve (ω_T) generated using HB scheme along with three different screening functions are shown in Fig. 2 and Fig. 3 for the $RE_{55}Al_{25}Co_{20}$ rare-earth bulk metallic glasses respectively. 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 understandable from the figures that the nature of peak positions are not much affected by different screening functions, but both the transverse and longitudinal frequencies show deviation by using T and F with respect to H screening functions. It is observed that the present fallout of phonon modes with correlation function due to T function is positioned between those due to H and F screening functions. The highest value of first peak point and lowest values of first peak point are seen for $Y_{55}Al_{25}Co_{20}$ and $Ce_{55}Al_{25}Co_{20}$ BMG respectively, and rest of rare earth bulk metallic glasses peak point fallout between these two bulk metallic glasses. It is clear from the figures that the oscillations are prominent in the longitudinal mode as compared to transverse mode, which indicates that the collective excitations at larger wave vector transfers due to the dispersion of longitudinal excitation. On the other hand the transverse modes undergo larger thermal modulation due to the anharmonicity of the vibrations in the bulk metallic glasses. In the long wavelength limit the dispersion curves are linear and confirming characteristics of elastic waves.

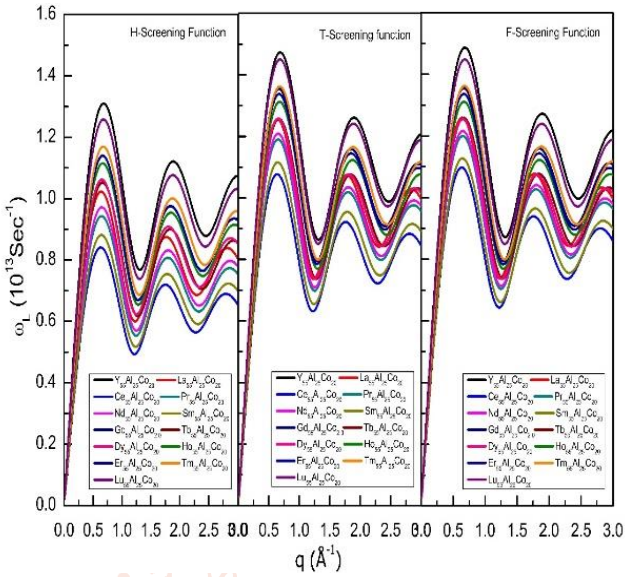

Fig.2 Screening dependence longitudinal collective modes of $RE_{55}Al_{25}Co_{20}$ BMG

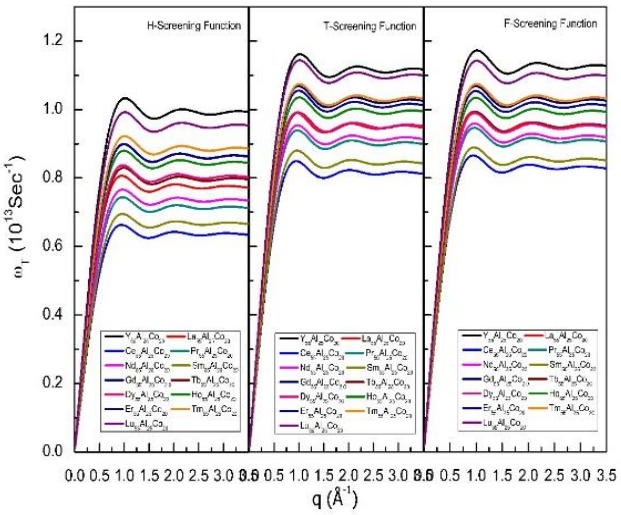

Fig.3 Screening dependence transverses collective modes of $RE_{55}Al_{25}Co_{20}$ BMG

Presently computed elastic properties for $RE_{55}Al_{25}Co_{20}$ rare-earth bulk metallic glasses are presented in Fig. 4 to Fig 10 for longitudinal sound velocity, transverse sound velocity, bulk modulus B_T, Poisson's ratio ν, modulus of rigidity G, Young's modulus Y and Debye temperature Θ_D along with experimental values respectively. The experimental values computed using the ultrasonic method is reported by W. H. Wang [3]. From these figures, one can see that the values are obtained due to T [16] and F [17] screening functions are very close to one another as compared to the H screening function. From the Fig 4 and Fig 5, the comparison shows that presently computed

results are obtain lower values for longitudinal velocity but better agreement with transverse sound velocity respectively. From Fig 6, one can see that outcome of bulk modulus show the underestimate computed using present model potential. But the F screening function shows the less deviation compared to H and T screening functions. From Fig. 5, Fig.7, Fig.8 and Fig.10 are shown the excellent agreement with available experimental values for transverse sound velocity, modulus of rigidity 'G', Young modulus 'Y' and Debye temperature Θ_D respectively. The experimental data are not available for $Y_{55}Al_{25}Co_{20}$, $Ce_{55}Al_{25}Co_{20}$, $Nd_{55}Al_{25}Co_{20}$, $Sm_{55}Al_{25}Co_{20}$ and $Gd_{55}Al_{25}Co_{20}$ bulk metallic glasses. So, at present we do not put any concrete remark for this bulk metallic glass. The computed elastic properties using T and F screening functions give excellent agreement particular for $Tb_{55}Al_{25}Co_{20}$, $Dy_{55}Al_{25}Co_{20}$ and $Ho_{55}Al_{25}Co_{20}$ bulk metallic glasses compare to in the series of other rare-earth bulk metallic glasses. From the Fig 4 to Fig 10 it is observed that the result generated due to HB-approach along with Jani et al model potential are found to be in acceptable agreement with the experimental results given in respective literatures.

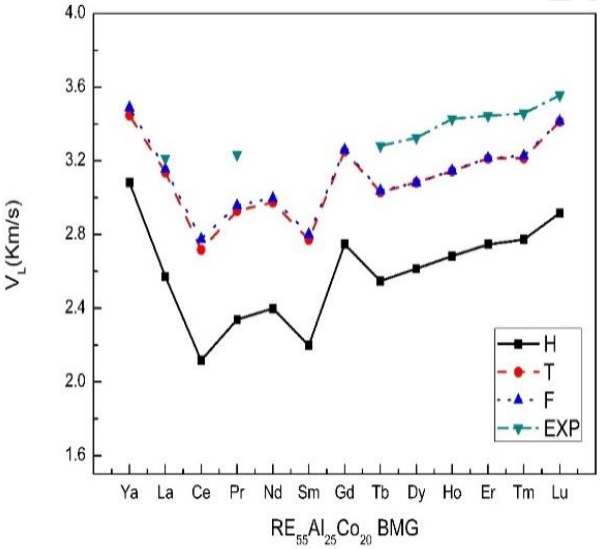

Fig.4 Longitudinal sound velocity (V_L) $RE_{55}Al_{25}Co_{20}$ BMG along with available experimental values [3]

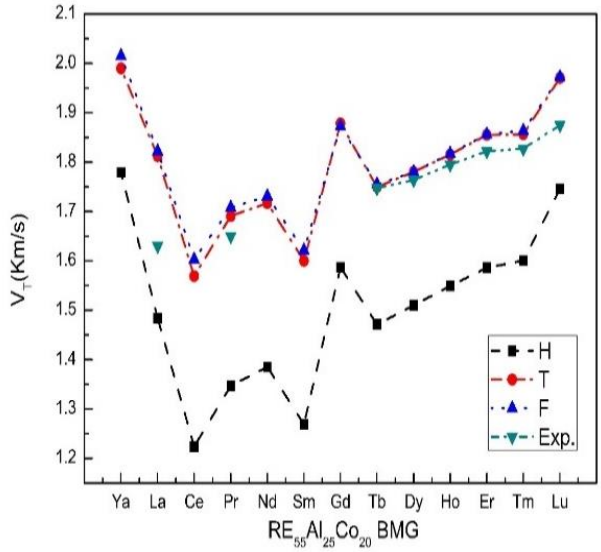

Fig.5 Transverses sound velocity (V_T) $RE_{55}Al_{25}Co_{20}$ BMG along with available experimental values [3]

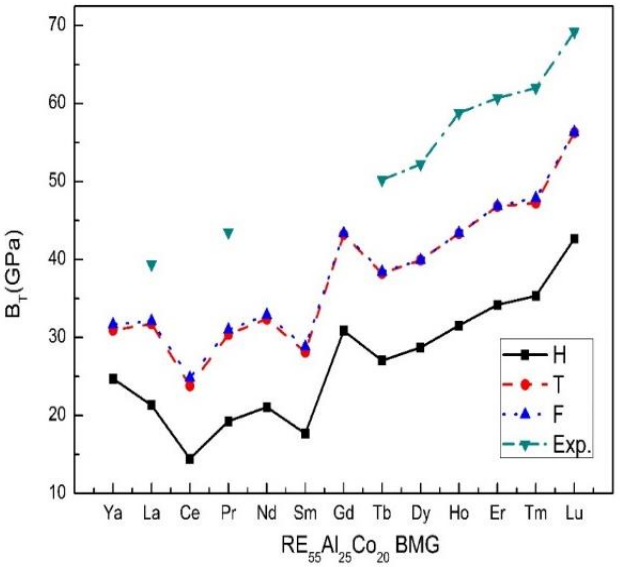

Fig.6 Bulk modulus (B_T) of $RE_{55}Al_{25}Co_{20}$ BMG along with available experimental values [3]

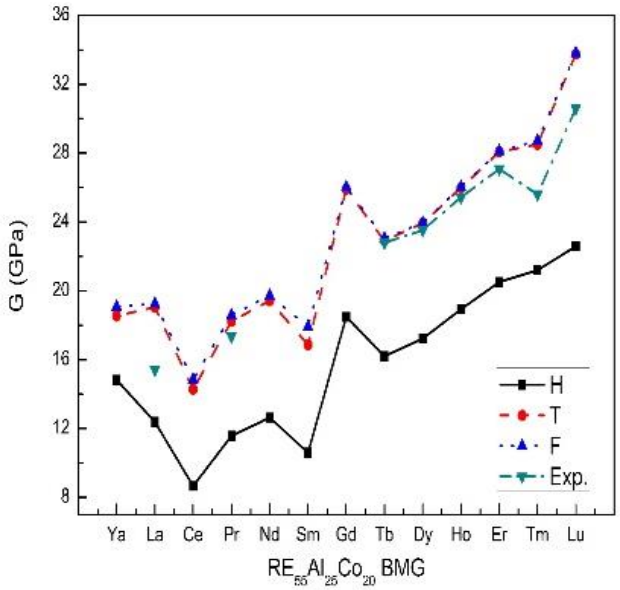

Fig.7 Modulus of rigidity (G) of $RE_{55}Al_{25}Co_{20}$ BMG along with available experimental values [3]

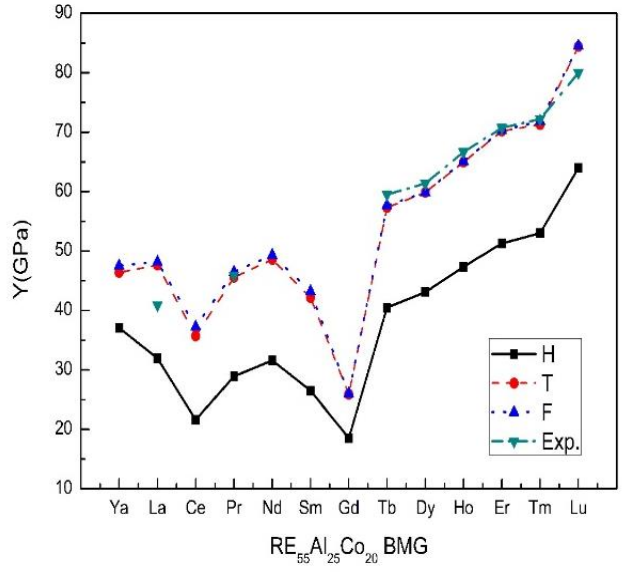

Fig. 8 Young's modulus (Y) of $RE_{55}Al_{25}Co_{20}$ BMG along with available experimental values [3]

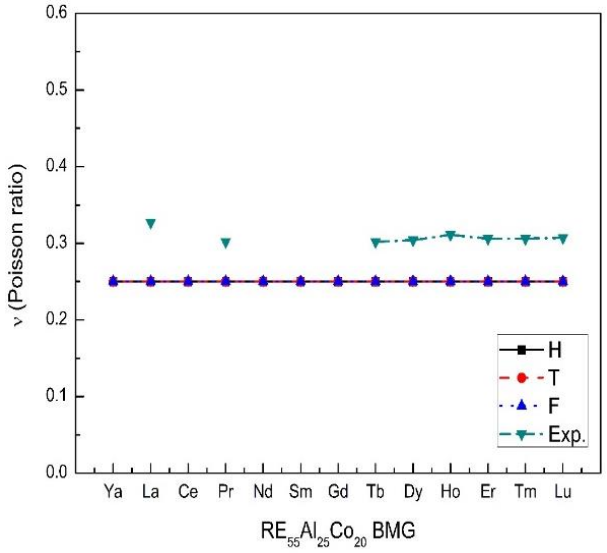

Fig.9 Poison ratio (υ) of $RE_{55}Al_{25}Co_{20}$ BMG along with available experimental values [3]

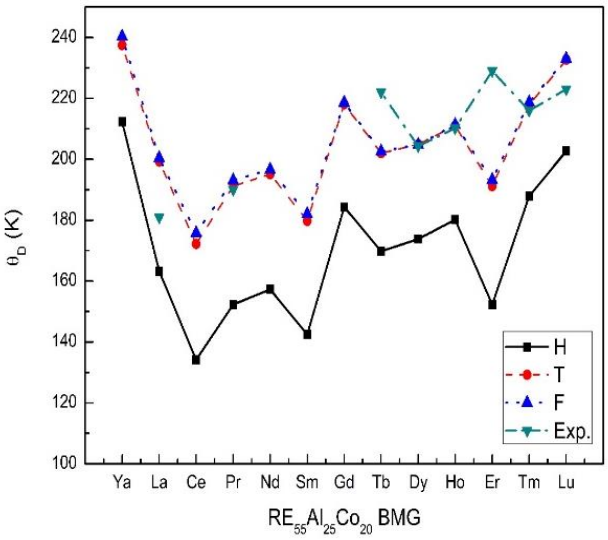

Fig.10 Debye temperature (Θ_D) of $RE_{55}Al_{25}Co_{20}$ BMG along with available experimental values [3]

TABLE II: $RE_{55}Al_{25}Cu_{20}$ percentile deviation with respect to experimental values

Elastic Properties	H [15]	T [16]	F [17]
Longitudinal sound velocity 'V_L'	17.96%-22.34%	2.33%-9.40%	1.77%-8.50%
Transverse sound velocity 'V_T'	6.89%-15.79%	0.14%-11.16%	0.45%-11.77%
Bulk modulus 'B_T'	38.35%-55.68%	18.68%-30.12%	18.56%-28.72%
Modulus of rigidity 'G'	17.18%-33.31%	0.52%-23.62%	1.14%-24.98%
Young modulus 'Y'	20.02%-36.99%	0.69%-16.22%	0.51%-17.74%
Poison Ratio 'υ'	18.30%-23.54%	18.3%-23.54%	18.30%-23.54%
Debye temperature Θ_D	9.10%-33.48%	0.29%-16.50%	0.24%-15.63%

The maximum and minimum percentile deviation of the various local field correlation functions with respect to the available experimental data is tabulated in Table 2. From this Table 2, the local field correction functions due to H (without exchange and correlation) give maximum percentile deviation compare to T and F functions and F functions gives the minimum deviation compare to other screening functions. So that we put the remark F screening function is very close to existing experimental data compared to H and T screening functions.

However, the improvement in the present finding may be achieved either by incorporating other forms of exchange and correlation effect or by suggesting the modification in determining the parameters of the potential. From this calculation, it is observed that the presently computed data serve as a guideline for further research in this direction.

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