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The Mechanic and Lattice Dynamical Properties on Stability of REMg (RE=Dy, Ho, Er) Alloys

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ABSTRACT

In this study, the the comprehensive investigation to structural, electronic, elastic, lattice dynamical properties of rare earth magnesium compounds REMg (RE= Dy, Ho, Er) were carried out using the density functional theory implemented in the projector-augmented wave (PAW) method. The calculated structural parameter in CsCl (B2) phase accords with experimental results. The elastic properties were caculated in a wide range of pressure (0-100GPa) for REMg (RE= Dy, Ho, Er). The calculated electronic band structure showed that these alloys have metallic character. The phonon dispersion curves and density of states (DOS) of REMg (RE= Dy, Ho, Er) which have not been calculated and measured yet, were also computed in CsCl phase using small displacement theory and found dynamically stable.

Keywords: magnesium alloys, mechanical properties, electronic structure, phonon

1. INTRODUCTION

Magnesium and its alloys have strong scientific and technological qualification especially automobile industry, space, aircraft and other applications [1-3]. Rare earth (RE)-magnesium (Mg) alloys considered in this work crystalize in CsCl structure[2-5]. Aleonard et al.[2] have performed neutron powder diffraction measurements for understanding the magnetic properties of rare earth magnesium compounds. Belakhovsky et al.[3] have also studied the magnetic properties of DyMg and ErMg using Mössbauer spectroscopy. In an early work, Buschow et al.[4] have analyzed the crystal structures and some physical properties of the intermetallic compounds of rare earths (from La to Lu) and non-magnetic metals (B, Be, Mg, Ru, Rh, Pd), experimentally. The crystal field parameters' of holmium compounds have reported by Scmitt et al [5].

Recently, Zhang et al.[6] have predicted the enthalpy of formation of MgX (X= As, Ba, Ca, Cd, Cu, Dy, Ga, Ge, La, Lu, Ni, Pb, Sb, Si, Sn and Y) compounds from the first-principles calculations. Wang et al. [7] have studied lattice dynamical and thermodynamic properties such as thermal expansions, bulk modulus, and heat capacities at constant volume and constant pressure as a function of temperature of rare-earth-magnesium intermetallic compounds MgRE (RE=Y, Dy, Pr, Tb) using both of density functional theory and density functional perturbation theory. They have also computed the temperature-dependent elastic properties and the second and third-order elastic constants from same family in B2-type structure [8,9]. Elastic and brittle properties have been investigated based on density functional theory for MgRE (RE = Sc, Y, Ce, Pr, Nd, Gd, Tb, Dy, Ho, Er) intermetallics in B2 structure and applying both the modified analytical embedded atom model and VASP package, the temperature dependence of thermodynamic properties and elastic constants of Mg-Pr, Mg-Dy, Mg-Y intermetallics are also estimated by Wu et al.[10,11].

Using an analytic modified embedded atom method the thermodynamic properties such as the dilute-limit heats of solution and enthalpies of formation of disordered

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solid solutions of Mg-RE (RE = Sc, Y, Pr, Nd, Gd, Tb, Dy, Ho or Er) system have been reported by Hu et al[12]. Recently, the generalized-stacking-fault energy (GSFE) surfaces for MgRE (RE=Y, Tb, Dy, Nd) intermetallics have also been studied by Wu et al[13], using the Vienna ab initio simulation package (VASP). Tao et al.[14] have focused phase stability and electronic properties of Mg–RE (RE = Sc, Y, and Lanthanide elements) binary systems from first principle calculation. They have calculated total energy, enthalpy of formation, equilibrium volume, bulk modulus, and electronic structure and found good agreement with experimental data. Tanh et al have studied the stacking faults of 17 B2 structured magnesium alloys systematically by using first-principles calculations. They have also investigated electronic structures to reveal the underlying mechanism for stability and stacking faults [15]. The structures and properties of <111>{110} superdislacations in B2-MgRE(RE= La-Er) intermetallics have been investigated using Peirles-Naborro model in combination with generalized stacking fault energies by Ma et al [16].

Despite numerous investigations [3-16] have been studied about Mg-RE alloy, the studies of RE-Mg systems are very limited. Here, we have focused on properties of REMg (RE= Dy, Ho, Er) compounds such as lattice dynamical and thermo-elastic properties under various pressures. To the best of our knowledge no theoretical study has yet been reported about structural, electronic, elastic and dynamical properties of REMg (RE= Dy, Ho, Er) compounds. It is well- known that elastic properties are essential fort the understanding of the macroscopic mechanical properties of REMg (RE= Dy, Ho, Er) alloys. Because they are related to various fundamental solid state and dynamical poperties. So in this work, we investigated structural, elastic, electronic and vibrational properties of REMg (RE= Dy, Ho, Er) alloys in B2 structure. We have also studied elastic constants and related other mechanical properties such as bulk modulus and shear modulus under pressure.

2. METHOD OF CALCULATION

In the present work, all the calculations were carried out using the Vienna ab initio simulation package (VASP)[17-20] based on the density functional theory (DFT). The electron–ion interaction was considered in the form of the projector-augmented-wave (PAW) method [19-21]. For the Exchange and correlation terms in the electron–electron interaction, Perdew and Zunger type functional [22,23] was used within the generalized gradient approximation (GGA) [22]. The 14x14x14 Monkhorst and Pack [24] grid of k-points was used for integration in the irreducible Brillouin zone. In each calculation the values of the k-point and the cutoff energy were selected in the range that guarantees the convergence of the total energy. This cut-off (650 eV) was found to be adequate for the structural, mechanical properties as well as for the thermodynamical ones. The total energy calculation was performed changing the unit cell volume using these selected values of k-point and cutoff energy. From the data set of total energy versus unit cell volume, the equilibrium lattice constant was easily derived from the Murnaghan Equation of State (EOS) method[25]:

$$E_{Tot} = E_0 + \frac{B_0 V}{B_0'}\left[\frac{\left(\frac{V_0}{V}\right)^{B_0'}}{B_0'-1} + 1\right] \quad (1)$$

Here, V, V_0, B_0 and B_0' are volume of unit cell, volume of unit cell at zero pressure, bulk modulus at zero pressures and pressure derivative of bulk modulus.

3. RESULTS AND DISCUSSION

3.1. Structural and electronic properties

The calculated equilibrium lattice constants, bulk modulus, and first pressure derivative of bulk modulus for REMg (RE= Dy, Ho, Er) compounds in the most probable NaCl (B1), CsCl (B2) and ZB (B3) structures were computed by minimizing the crystal total energy calculated for different values of lattice constant by means of Murnaghan's equation of state (EOS) [25] . Our calculated values are shown in Table 1 with the other experimental data [2, 26] for considered phases. The present values of lattice parameter are, only, overestimated as ~0.5% for DyMg and ErMg, 0.32% for HoMg compared to Ref [24] and ~0.26, 0.16 and 0.21% compared to Ref. [2] for REMg (RE= Dy, Ho, Er) compounds, respectively, thus it strongly supports the choice of pseudopotentials (i.e. GGA approximation) for the current study.

The calculated results of formation energies are also displayed in Table 1. Formation energies in a given phase is defined as the difference in the total energy of the constituent atoms at infinite separation and the total energy of that particular phase:

$$\Delta H^{REMg} = E_{total}^{REMg} - [E_{solid}^{RE} + E_{solid}^{Mg}] \quad (2)$$

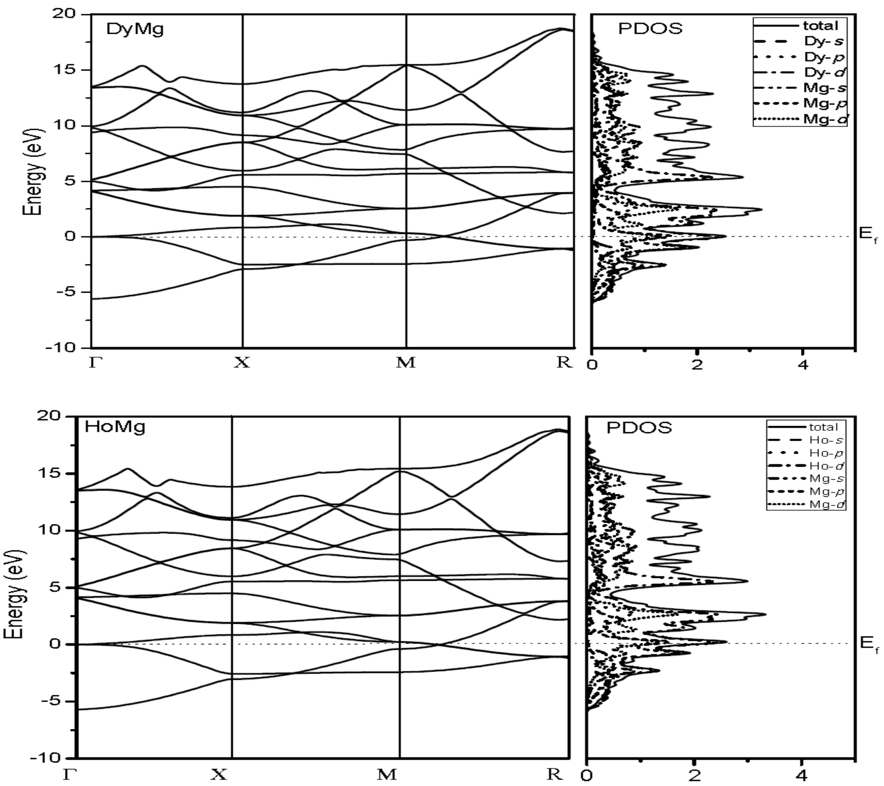
where E^{REMg}_{total} is the total energy (in formula unit) of the compounds at equilibrium lattice constant and E^{RE}_{solid} and E^{Mg}_{solid} are the atomic energies of the pure constituents. The computed formation energies (ΔH) are found to be -0.159, -0.141, -0.108 eV/f.u in B2 structure for REMg (RE= Dy, Ho, Er), respectively. These results denote the thermodynamic stability of these compounds for only B2 structure, indicating these materials might be easily synthesized experimentally in B2 structure. Due to formation energies are positive, the compounds are thermodynamic unstable in B1 and B3 structures.

In order to further understand of the electronic behavior of these compounds, we have investigated the electronic band-structure calculations for B2 structure, and the present results for both the band structures and partial and total density of states are given in Figure 2. The position of Fermi level is at 0 eV. It is clearly seen from these figures that no band gap exists for each compounds, and they exhibit metallic character. Largest contribution comes from RE d-states to the total density of states at the Fermi level with minor presence RE-s and Mg-p states. The RE-p and Mg-p states are also contributing to the bands. It is seen from Fig. 2a-c that REMg (RE= Dy, Ho, Er) have very similar band structures curves and the corresponding density of states except a little differences. The disappearing of the energy gap in DOS confirms the metallic nature of REMg (RE= Dy, Ho, Er).

Table 1. Calculated equilibrium lattice constants(a_0), bulk modulus (B), pressure derivatives of bulk modulus (B′), formation energy (ΔH) and other experimental studies for REMg (RE= Dy, Ho, Mg)

Materials	Structure	Reference	a_0 (Å)	B(GPa)	B′	H (eV/f.u.)
DyMg	B2	Present (GGA)	3.778	40	3.36	-0.159
		Exp.[a]	3.759			
		Exp.[b]	3.768			
	B1	Present (GGA)	6.242	33.794	3.7	0.793
	B3	Present (GGA)	7.068	14.63	3.58	2.46
HoMg	B2	Present (GGA)	3.767	39.734	3.465	-0.141
		Exp.[a]	3.755			
		Exp.[b]	3.761			
	B1	Present (GGA)	6.217	33.754	3.75	0.815
	B3	Present (GGA)	7.065	14.5	3.56	2.475
ErMg	B2	Present (GGA)	3.756	40.06	3.478	-0.108
		Exp.[a]	3.737			
		Exp.[b]	3.748			
	B1	Present (GGA)	6.194	33.617	3.81	0.869
	B3	Present (GGA)	7.063	14.387	3.543	2.516

[a] : [25], [b] : [2]



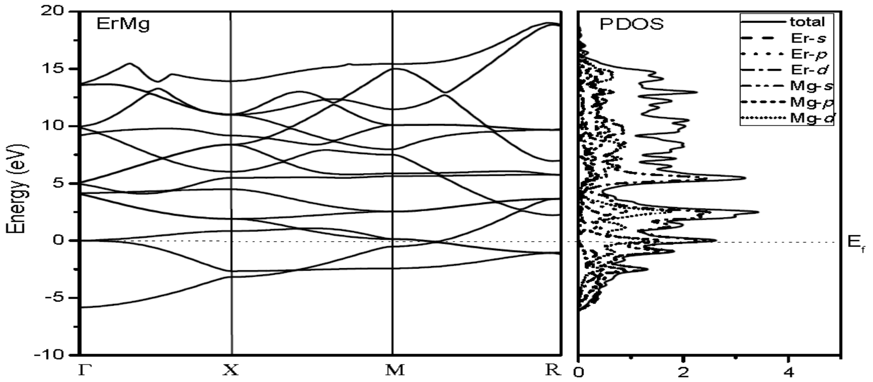


Fig 1. Calculated band structure and partial density states (PDOS) for REMg (RE=(a) Dy, (b) Ho, and (c) Er) in phase B2.

3.2. Mechanical properties

The elastic constants of solids provide a link between the mechanical and dynamical behaviour of crystals, and give important information concerning the nature of the forces operating in solids. In particular, they provide information on the stability and stiffness of materials. Their ab-initio calculation requires precise methods, since the forces and the elastic constants are functions of the first and second-order derivatives of the potentials. Their calculation will provide a further check on the accuracy of the calculation of forces in solids. The effect of pressure on the elastic constants is essential, especially, for understanding interatomic interactions, mechanical stability, and phase transition mechanisms. Here we have used the "stres-strain" relation [27, 28], for obtaining the second-order elastic constants (C_{ij}).

The method is based on constructing a set of linear equations from stress-strain relationships for several deformations of the unit cell. This set of equations represents a general form of the Hook's law and can be solved with respect to the elastic constants. Since in practice this set of equations is overdetermined, to solve it we have used a singular value decomposition algorithm which automatically provides a least squares solution of the set [29]. The calculated values for C_{ij} are listed in Table 2. For cubic system the mechanical stabilitiy conditions can be expressed as follow:

$C_{11} - C_{12} > 0$ $C_{11} > 0$ $C_{44} > 0$ $C_{11}+2C_{12} > 0$ $C_{12} < B < C_{11}$.

Table 2. The calculated elastic constants (in GPa unit) with Zener anisotropy factor (*A*), Poisson ratio (*v*), Young's modulus (*Y*) and isotropic Shear modulus (G) in B2 structure

Material	C_{11}	C_{12}	C_{44}	C_{12}-C_{44}	A	υ	Y	G
DyMg	52.33	37.05	40.37	-3.32	5.29	0.276	53.79	21.08
HoMg	52.0	37.93	40.79	-2.86	5.8	0.279	52.76	20.63
ErMg	52.19	38.66	41.58	-2.92	6.14	0.280	52.82	20.62

As shown in Table 2, the elastic constants provide with all these stability criteria. Therefore we can say that these three compounds are elastically stable in B2 structure. We have evaluated the brittle/ductile behaviour of these compounds using the Cauchy pressure condition. The positive Cauchy pressure is corresponded ductile characteristic while negative Cauchy pressure point out brittle characteristic [30]. It is noticable that REMg (RE= Dy, Ho, Er) compounds exhibit brittle behavior at low pressure and ductile behavior at high pressure. The other commonly used empirical relations between bulk and isotropic shear modulus for covalent and ionic materials on their brittle/ ductile behavior are G~1.1B and G~0.6B, respectively [31, 32]. The present values of G/B are 0.527, 0.519 and 0.515 for REMg (RE= Dy, Ho, Er), respectively at zero pressure and they are higher than the critical value of 0.5. These results also support their ionic and brittle character. Due to ductile nature G/B are less than the 0.5 at high pressure.

The pressure dependence of elastic constants are calculated and shown in Figure 3. As expected, C_{ij} increase almost monotonically with pressure up to the considered pressure (100 GPa). Although there are no available values to compare with our calculated results, our data will be beneficial to future investigations. It has been found that C_{11} varies substantially under the pressure when compared with the variations in C_{12} and C_{44}.

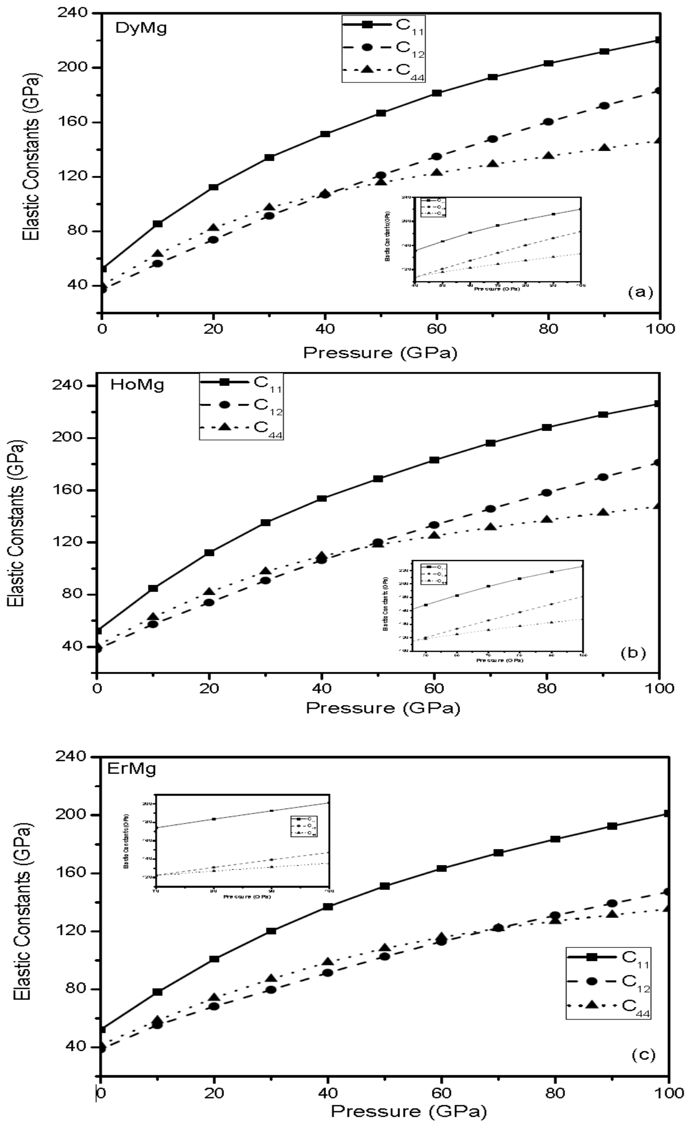


Fig 2. The pressure effect of elastic constants for REMg (RE=(a) Dy, (b) Ho, and (c) Er) in B2 structure

The Zener anisotropy factor *A*, Poisson ratio υ, and Young's modulus *Y*, which are the most interesting elastic properties for applications, are also calculated in terms of the computed data using the following relations [33] :

$$A = \frac{2C_{44}}{C_{11} - C_{12}}, \tag{3}$$

$$\upsilon = \frac{1}{2}\left[\frac{(B - \frac{2}{3}G)}{(B + \frac{1}{3}G)}\right], \tag{4}$$

and

$$Y = \frac{9GB}{G + 3B} \tag{5}$$

where $G = (G_V + G_R)/2$ is the isotropic shear modulus, G_V is Voigt's shear modulus corresponding to the upper bound of G values, and G_R is Reuss's shear modulus corresponding to the lower bound of G values, and can be written as $G_V = (C_{11}–C_{12} + 3C_{44})/5$, and $5/G_R = 4/(C_{11}-C_{12}) + 3/C_{44}$. The calculated elastic constants, Zener anisotropy factor (*A*), Poisson ratio (υ), Young's modulus (*Y*), and Shear modulus ($C' = (C_{11}-C_{12}+2C_{44})/4$)

for REMg (RE= Dy, Ho, Er) are given in Table 2. The pressure dependence of the bulk (B), young(Y), and shear (G) modulus are plotted in Figure 3. It is seen from these figures that the bulk modulus increases linearly with pressure for three compounds. But the increasing in Young and shear modulus with pressure is gradual and their slope is lower.

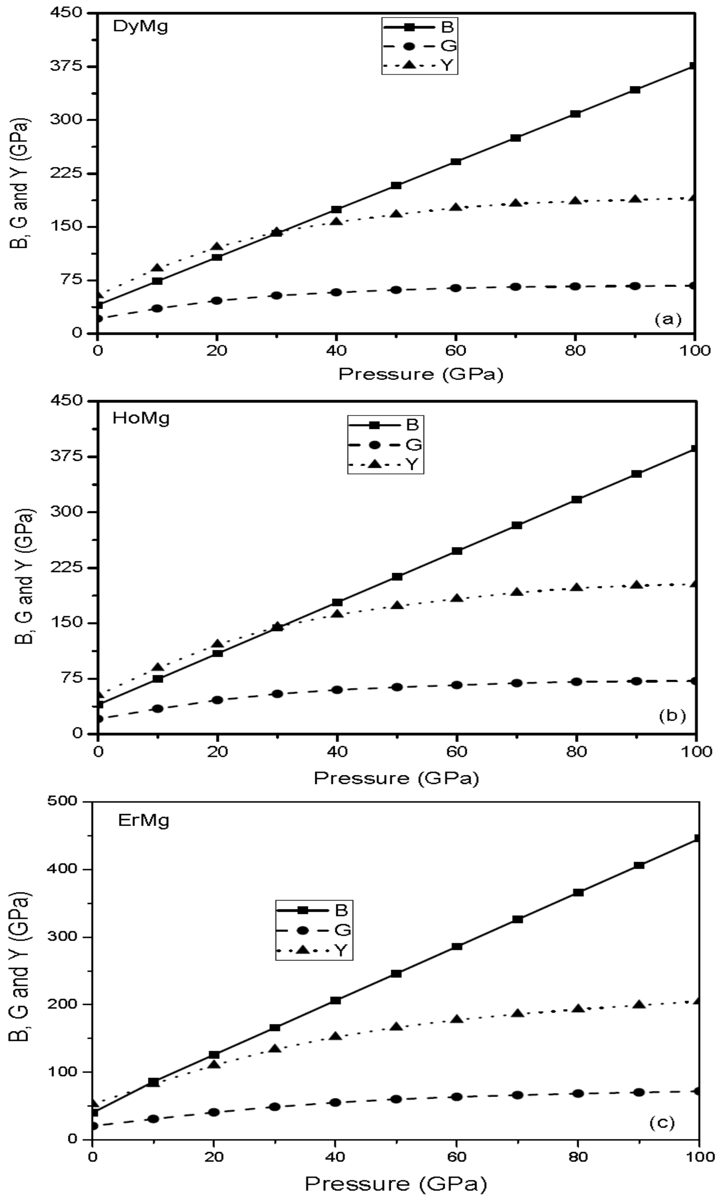


Fig 3. The *B* (bulk modulu), *Y* (Young modulu), *G* (Shear modulu) as a function of pressure for REMg (RE=(a) Dy, (b) Ho, and (c) Er) in B2 structure.

The Zener anisotropy factor *A* is a measure of the degree of elastic anisotropy in solids. The *A* takes the value of 1 for a completely isotropic material. If the value of *A* smaller or greater than unity it shows the degree of elastic anisotropy. The calculated Zener anisotropy factors for REMg (RE= Dy, Ho, Er) are equal to 5.29, 5.8 and 6.14 respectively, which indicates that these compounds are completely anisotropic materials.

The Poisson's ratio υ and Young's modulus *E* are very important properties for industrial applications. The Poisson's ratio υ provides more information about the characteristics of the bonding forces than any of the other elastic constants. The lower limit and upper limit of Poisson's ratio υ are given 0.25 and 0.5 for central forces in solids, respectively[34]. Calculated υ values are equal to 0.276, 0.279 and 0.280 for REMg (RE= Dy, Ho, Er) , respectively. It shows that, the interatomic forces in the REMg (RE= Dy, Ho, Er) are central forces. The Young's modulus *E*, the ratio between stress and strain, is required to provide information about the measure of the stiffness of the solids. The present values of Young's moduli decrease from DyMg to HoMg, which points out that DyMg is stiffer than HoMg and ErMg.

The Debye temperature (θ_D) is known as an important fundamental parameter closely related to many physical propertied such as specific heat and melting temperature. At low temperatures the vibrational excitations arise solely from acoustic vibrations. Hence, at low temperatures the Debye temperature calculated from elastic constants is the same as that determined from specific heat measurements. We have calculated the Debye temperature, θ_D, from the elastic constants data using the average sound velocity, v_m, by the following common relation [35].

$$\theta_D = \frac{h}{k}\left[\frac{3n}{4\pi}\left(\frac{N_A\rho}{M}\right)\right]^{1/3}\upsilon_m \qquad (6)$$

where $\hbar$ is Planck's constants, k is Boltzmann's constants, N_A Avogadro's number, n is the number of atoms per formula unit, M is the molecular mass per formula unit, $\rho(=M/V)$ is the density, and v_m is obtained from [36]

$$\upsilon_m = \left[\frac{1}{3}\left(\frac{2}{\upsilon_t^3}+\frac{1}{\upsilon_l^3}\right)\right]^{-1/3} \qquad (7)$$

where v_l and v_t, are the longitudinal and transverse elastic wave velocities, respectively, which are obtained from Navier's equations [37]:

$$\upsilon_l = \sqrt{\frac{3B+4G}{3\rho}} \qquad (8)$$

And

$$\upsilon_t = \sqrt{\frac{G}{\rho}}\ . \qquad (9)$$

The calculated average longitudinal and transverse elastic wave velocities, Debye temperature and melting temperature for REMg (R= Dy, Ho, Er) are given in Table 3. No other theoretical or experimental data are exist for comparison with the present values.

Table 3. The longitudinal, transverse, average elastic wave velocities, and Debye temperature for REMg (RE= Dy, Ho, Mg) in B2 structure.

Material	$\upsilon_l\,(m/s)$	$\upsilon_t\,(m/s)$	$\upsilon_m\,(m/s)$	$\theta_D\,(K)$	$T_m\,(K)$
DyMg	1720.1	956.9	1065.67	166.04	862.29± 300
HoMg	1690.74	936.5	1043.276	164.9	1052.92± 300
ErMg	1677.12	926.64	1032.5	165.57	861.45± 300

3.3. Phonon Dispersion Curves

The present phonon frequencies of REMg (RE= Dy, Ho, Er) compounds in B2 phase are calculated using the PHON code [38] based on the forces obtained from the VASP. The PHON code calculates force constant matrices and phonon frequencies using the "Small Displacement Method" as described in References [39, 40]. Specifically, the phonon dispersion curves and one-phonon density of state have been calculated in high symmetry directions using a 2x2x2 cubic supercell of 16 atoms. The obtained results along the high symmetry directions are illustrated in Fig. 4. To our knowledge there are no experimental and other theoretical works exploring the lattice dynamics of these compounds for comparison with the present data; hence our work is a first attempt in this direction. The obtained frequencies at the high symmetry points Γ and X are given in Table 4. The absence of the negative frequencies in the phonon dispersion curves in Fig.4, strongly supports the dynamical stability of these compounds in B2 phase. Owing to the mass difference between RE (R= Dy, Ho, Er) and Mg atom the large band gap takes place between acoustic and optical regions. As is expected, the overall shapes of the dispersion curves and the related one-phonon density of states resemble to each other for three compounds with small differences.

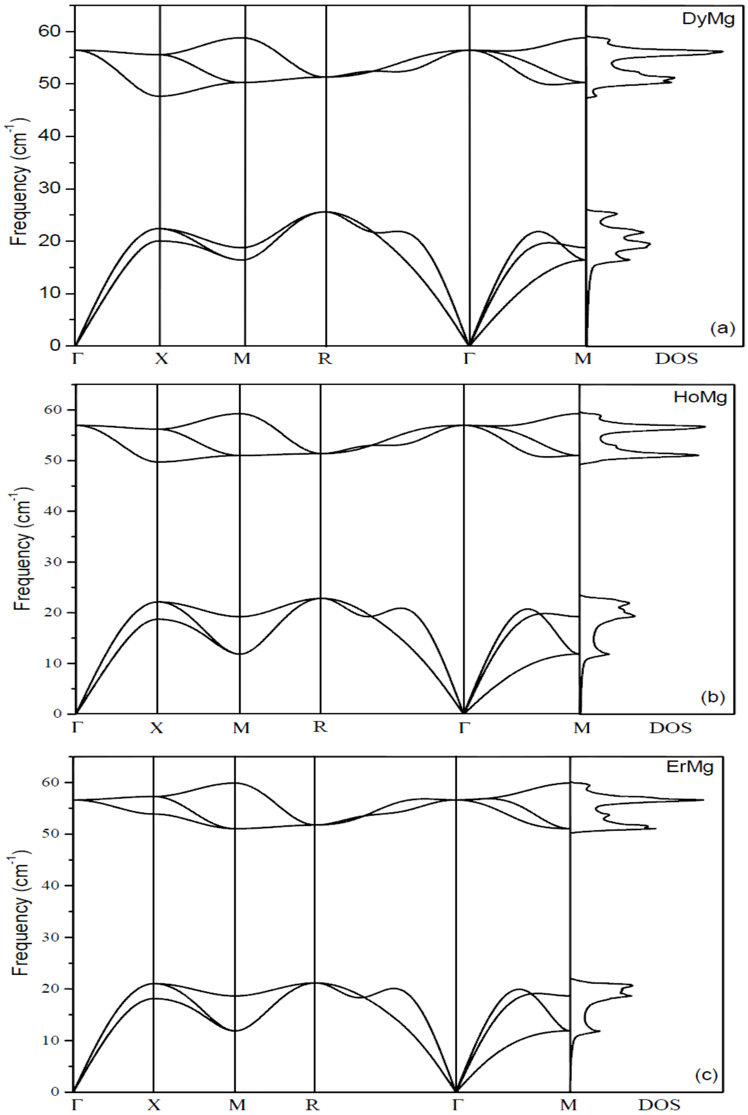


Fig 4. Calculated phonon dispersions and total density of states for REMg (RE=(a) Dy, (b) Ho, and (c) Er) in B2 structure.

Table 4. Phonon frequencies (in cm^{-1}) of REMg (RE= Dy, Ho, Mg) at the Γ and X points.

Material	TA(X)	LA(X)	T0(X)	LO(X)	T0(Γ)	LO(Γ)
DyMg	20.09	22.365	47.715	55.6	56.365	56.365
HoMg	18.58	22	51.22	59.25	57.1	57.1
ErMg	18.1	21	53.93	57.27	56.526	56.526

4. SUMMARY AND CONCLUSION

Using first principle calculation, we obtained many practical structural, elastic, electronic, and lattice dynamical results for REMg (RE= Dy, Ho, Er) intermetallic compounds. The lattice parameters are in excellent agreement with the other experimental findings in B2 structure. Some of basic results such as second-order elastic, Zener anisotropy factor, Poisson's ratio, Young's modulus, longitudinal, transverse and average elastic wave velocities and Debye temperatures are also reported here. These compounds are displayed metalic and brittle characteristic at zero pressure. The electronic band structures, phonon dispersion curves and densities of states for each compound have been denoted. The band structures and phonon dispesion curves exhibite similar behaviour for three compounds. It is hoped that some our results such as calculated elastic constants and vibrational frequencies will be helpful in future experimentally and theoretically.

CONFLICT OF INTEREST

No conflict of interest was declared by the authors.

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