The full-potential study of ErMg

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Abstract. The structural, electronic and magnetic properties of ErMg are investigated using the full potential linear augmented plane wave method based on density functional theory. The calculated structural parameters using LDA are in excellent agreement with the available experimental result. The calculated band structure is at 0 GPa. The valence and conduction bands are overlapped notable at the Fermi level ($E_F = 0$ eV). Consequently, there is no energy gap. The calculated band structure shows that this alloy has metallic nature. Total magnetic moment at equilibrium lattice constant of ErMg intermetallic in B2 phase along with the magnetic moment on the atomic and interstitial sites have also been presented in this paper.

1. Introduction
Magnesium is a superb metal because it is readily available and it is the lightest of all the structural metals having a density of 1.7g/cm$^3$. Magnesium mostly found in the earth’s ocean. Magnesium has hexagonal close packed crystal structure. Therefore the property of deformation is difficult in such type of alloy. This structure restricts its ability to deform because it has fewer slip systems at lower temperatures. Magnesium has low melting point. Due to this property make easier to melt for casting. Pure magnesium is rarely used in the manufacturing of aerospace and automotive parts. In order to make use in developing purpose, magnesium is alloyed with other metals. Most common alloyed elements in commercial alloys are: aluminum, zinc, cerium, silver, and thorium. Magnesium can also be alloyed with rare earth elements, which increase the strength of magnesium especially at high temperature. The significant properties of magnesium alloys are light weight, low density (two thirds that of aluminum), and have good high temperature mechanical properties with good to excellent corrosion resistance. Magnesium alloys are good for engineering applications because they have good strength, ductility and creep properties. Magnesium alloys have replaced engineering plastics in many applications because they have a comparable density but are stiffer, more recyclable and less costly to produce. Magnesium is strong and light, making it an excellent choice for aerospace applications. Magnesium is also used in other products such as hand-held devices (chain saws, power tools, hedge clippers), in automobiles (steering wheels and columns, seat frames, transmission cases, crank case, camshaft sprocket, gearbox housings), and in audio-video-computer-communications equipment (laptop computers, camcorders, TV sets, cellular telephones). The Mg-RE based alloys serve a useful purpose in automotive industry as superior light metal-alloys in cast or wrought condition [1]. Mg-RE alloys also gained prominence in biomedical applications [2]. To recognize the magnetic properties of rare earth magnesium alloy Aleonard et al. [3] have performed neutron powder diffraction measurement. The magnetic properties of DyMg and ErMg using Mossbauer spectroscopy are also studied by Belakhovsky et al. [4]. In an early work, Buschow et al. [5] have analyzed the crystal structures and some physical properties of the intermetallics compounds of the rare earth (from La to
Lu) and non magnetic metals (B, Be, Mg, Ru, Rh, Pd) experimentally. The magnetic properties of rare earth magnesium compounds with CsCl structure have been determined in the temperature range 4.2 to 300K by Buschow et al [6] and also reported by Kirchmayr at etal. [7]. Zhang et al. [8] have predicted the enthalpy of formation of MgX (X =As, Ba, Ca, Cd, Cu, Dy, Ga, Ge, La, Ni, Lu, Pb, Si, Sn and Y) compounds from the first –principles calculation. The Brittle and elastic properties of the MgRE (RE= Sc, Y, Pr, Nd, Dy, Ho, Er) in CsCl structure have been investigated using the first principles density functional calculation by Wu and Hu [9]. The intermetallics phases in their hand book of crystallographic data are presented by Villars et al. [10]. The elastic properties of B2-MgRE (RE=Sc, Y, La–Lu) intermetallics have been calculated at T=0K by using first principles within the generalized gradient approximation (GGA) by Tao et al. [11]. Wang et al. [12] have studied lattice dynamical and thermodynamic properties such as thermal expansion, bulk modulus, heat capacities at constant volume and constant pressure as a function of temperature of the rare earth magnesium intermetallics compounds MgRE (RE=Y, Dy .Pr, Tb) using density functional theory (DFT). They have also computed the temperature-dependent elastic properties and second and third order elastic constants for same family in CsCl type structure.In this paper, we have presented the structural, electronic and magnetic properties of ErMg alloy by using the wien2k code, theoretically.

2. Computational details
The zero-temperature energy calculations are performed using both the all-electron full-potential linear augmented-plane-wave method (FP-LAPW). All the calculations have been carried out using the WIEN2k code [13]. The sphere radii used in the calculations are 3.0 and 2.2 a.u. for Er and Mg, respectively. Within these spheres, the charge density and potential are expanded in terms of crystal harmonics up to angular momenta l = 10, and a plane wave expansion has been used in the interstitial region. The Brillouin zone integrations for the total energy are performed using both the all-electron full-potential linear augmented-plane-wave method (FP-LAPW). All the calculations have been carried out using the WIEN2k code [13]. The sphere radii used in the calculations are 3.0 and 2.2 a.u. for Er and Mg, respectively. Within these spheres, the charge density and potential are expanded in terms of crystal harmonics up to angular momenta l = 10, and a plane wave expansion has been used in the interstitial region. The Brillouin zone integrations for the total energy have been carried out using 35 special k-points in the irreducible Brillouin zone. Well converged solutions were found for R_{cut}=7, where K_{max} is the plane wave cut-off and R_{cut} is the atomic sphere radii. Both the muffin-tin radius and the number of k-points are varied to ensure convergence. Core states are treated fully relativistic but for valence states relativistic effects have been included in a scalar relativistic treatment. The self-consistent calculation stops only when the total energy and the charge of the system meet the convergent limit of the order 10^{-4} Ry and 10^{-3} e', respectively. The equilibrium lattice constant was obtained by fitting the total energy versus volume according to the Murnaghan equation of states [14].

3. Results and discussions

3.1 Structural properties
The equilibrium lattice parameters are determined by the energy minimization procedure. As a first step, a set of the unit cell volume and total energy is calculated using local density approximation (LDA). At the equilibrium volume, we set the atomic positions to obtain the equilibrium structure of the unit cell. The results thus achieved are operated to obtain a new set of the total energy and the unit cell volume, which are used to obtain equilibrium bulk modulus and its pressure derivative using the Murnaghan equation of states. The obtained results are shown in table 1. From table 1, it can be seen that the calculated lattice constants using the LDA formalism are consistent with the available experimental results.

**Table 1.** Calculated lattice constant, a(Å), the bulk modulus B_0 (GPa), bulk modulus first pressure derivative B'_0 and total energy E_0 (Ry) of ErMg along with the available theoretical and experimental data in B2 phase.

| Material | Phase | a (Å) | B_0 | B'_0 | E_0 (Ry) | Ref. |
|----------|-------|-------|-----|------|---------|-----|
| ErMg     | B2    | 3.72  | 35.96 | 3.96 | -26582.03 | P.W |
|          |       | 3.74  | -    | -    | -       | Exp.[3] |
|          |       | 3.75  | 40.06 | 3.47 | -       | The. [15] |
3.2 Electronic properties
The self-consistent band structures of ErMg were calculated in B2 phase at equilibrium lattice constant within the LDA scheme in spin up and spin down case. The overall profile of band structures in spin up and spin down cases show the metallic character. The obtained band structures are good agreement with the available data. But in spin up case the band is shifted towards the Fermi level. The obtained band structures are shown in Figure 2.

3.3 Density of states
To understand the behaviour of electronic band structure, we have plotted the total density of states (TDOS) and partial density of states (PDOS) in spin and spin down case. In case of TDOS, it seems the bands lie within the region -2.0eV to -4.0eV is due to the main contribution from Er- 4f states. Peaks are concentrated in the range -2.0 to –4.0eV in spin up cases while in spin down cases f states overlap Fermi level completely from 1.0eV to -1.0eV. The contribution of Mg-s states in band formation are also shown in figure 3.

3.3 Magnetic properties
Magnetic moment of any compound play very important role to identify the internal contribution of the spin of the electrons. The spin polarized self-consistent band structure calculation has been very successful in predicting the magnetic moment by LDA scheme. The obtained value of magnetic moments of ErMg in B2 phase is listed in Table 2. It is clear that the total and local magnetic moments (M and m) decrease with the increase in lattice parameter. The main contribution to the magnetic moment is mainly due to the 4f electrons of Er, while the contribution of Mg almost negligible. The magnetic moment Mg atom is negative, which specify that the involvement of 2p states of Mg atom is anti-parallel to that of Er.
Table 2. Obtained values of atomic and total spin magnetic moments of ErMg in stable CsCl phase

| Lattice parameter | m_{Er} | m_{Mg} | m_{int} | Total  |
|------------------|--------|--------|---------|--------|
| 6.80             | 2.3531 | -0.0203| -0.0972 | 2.2355 |
| 6.92             | 2.3533 | -0.0182| -0.0922 | 2.2428 |
| 7.04             | 2.3490 | -0.0165| -0.0893 | 2.2432 |
| 7.16             | 2.3428 | -0.0151| -0.0875 | 2.2402 |
| 7.27             | 2.3343 | -0.0142| -0.0891 | 2.2309 |

Figure 3. Spin-dependent total (a) and partial (b), (c) density of states of ErMg, using LDA scheme.

4. Conclusions

The structural, electronic and magnetic properties of ErMg intermetallic alloy are investigated by employing the first principles FP-LAPW based on DFT. The obtained equilibrium structural parameters are in excellent agreement with the experimental ones and also are served in this work to study the other properties. The electronic band structure results show that this alloy has metallic nature and the density of states also indicate that there is no gap at Fermi level. The total and local magnetic moment decrease with the increase lattice parameter. Rare earth atom i.e. Er show the main contribution in total magnetic moment due to 4f electrons. Negative sign of Mg atom specify that antiparallel spin to that of Er.

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