Advances in Physics Theories and Applications
ISSN 2224-719X (Paper) ISSN 2225-0638 (Online)
Vol.19, 2013 - Selected from International Conference on Recent Trends in Applied Sciences with Engineering Applications
www.iiste.org

Ab-initio Study of Structural, Electronic and Elastic Properties of ErCu

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Abstract
First principles density functional calculations were performed to study the structural, electronic, elastic and mechanical properties of erbium copper intermetallic compound (ErCu). The calculations are carried out within the generalized gradient approximation (GGA) for the exchange and correlation potential. The total energy as a function of volume is obtained by performing spin-polarized calculation. Magnetically the ErCu compound is stable in ferromagnetic (FM) state and its crystal structure is CsCl-type. Ground state properties such as lattice constant (a_0), bulk modulus (B), its pressure derivative (B′) and magnetic moment (μ_B) are calculated. The density of states at the Fermi level, $N(E_F)$ and specific heat coefficient are also estimated in majority and minority spin channels. The electronic properties such as band structure and density of states (DOS) reveal that no band gap lead to metallic character of ErCu. The elastic constants (C_{11}, C_{12} and C_{44}) and mechanical properties such as Poisson's ratio (σ), Young's modulus (E), shear modulus (G_H), anisotropic factor (A) are also calculated . Ductility for these compounds is further analyzed by calculating the ratio of (B/G_H) and Cauchy pressure (C_{12} - C_{44}).
Keywords: Density functional theory, Band structure, Density of states, Lattice constant, Bulk Modulus, Specific heat

1. Introduction

The intermetallic compounds are described as possessing "mixed bonding" and exhibit a diverse range of fascinating chemical, electrical, physical, magnetic and mechanical properties that are superior to ordinary metals [1]. Intermetallic compounds exhibit the best combination of low density, high oxidation resistance, high stiffness and high strength, but their enormous potential for improving engineering performance remains largely unused because they are brittle and fracture easily at room temperature [2]. The binary B_2 intermetallic compounds are inherently brittle, but recently a new class of ductile RM (where R= a rare earth and M= transition metal) have been discovered by Gschneidner *et al.* [3]. Some RM intermetallic compounds have been found to be highly ductile and thus has moved the horizon of fracture toughness and other mechanical properties of the intermetallic compounds is under crucial investigation. ErCu possess unusually high ductility and crystallizes in the cubic type structure (B_2, Pm3m, space group no. 221) in which the Er atom occupy the corner atoms of a cube and Cu atom are in the body centered site. There are a number of rare earth intermetallics that have CsCl type structure and have been studied experimentally [4,5]. Sekkal *et al.* [6] have investigated the structural, elastic and thermal properties of intermetallic B_2-YX (X = Cu, Mg and Rh) compounds using full-potential augmented plane wave method within the generalized gradient approximation. The electronic structure, elastic constants, lattice dynamics of the B2 type intermetallic compound LaAg are studied by means of density functional theory by Vaitheeswaran *et al*. [7]. The first principles calculations were used to study the mechanical and electronic properties of AgRE satisfactorily by Xiaoma *et al.* [1]. The interest in theoretical calculation of crystalline electric field (CEF) on the *'f'* electrons of rare earth (RE) ion in intermetallic compound comes from the fact that CEF on *'f'* electron is very important to the magnetic properties of the compound. Morin *et al.* [8] have determined CEF parameter for ErX (X=Cu, Ag, Zn, Mg, Pd) by inelastic neutron scattering experiment. Magnetic and structural characteristics of LnCu were explored by Walline *et al.* [9].
The aim of the present paper is to investigate the ground state, electronic and elastic properties of ErCu by using density functional theory and thus to gain a deeper understanding of the material and their potential applications. Remaining part of the paper is organized as follows: Section 2 describes the method of calculation. Section 3 is

the result followed by the discussion. Section 4 is the conclusion.

2. Method of calculation

The calculations have been performed in the frame work of density functional theory (DFT). We have used the full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2K code [10]. The exchange and correlation effects were treated using the (GGA) approximation [11]. In order to achieve convergence, we expand the basis function up to $R_{MT}*K_{max}$ =7 where R_{MT} is the smallest atomic radius in the unit cell and K_{max} gives the magnitude of the largest ***k*** vector in the plane wave expansion. The maximum value for partial waves inside the atomic sphere is l_{max} = 10 while the charge density is Fourier expanded up to G_{max} = 12. The self-consistent calculations are converged when the total energy of the system is stable within 10^{-4} Ry. A dense mash of 1000 ***k*** points and the tetrahedral method [12]. have been employed for the Brillouin zone integration. The calculated total energies are fitted to the Birch-Murnaghan equation of state[13] to determine the ground state properties like lattice constant (a_0), bulk modulus (B) and its pressure derivative (B′) at minimum equilibrium volume V_0.

$$E(V) = E_0 + \frac{BV}{B'}\left[\frac{(V_0/V)^{B'}}{(B'-1)}+1\right] - \frac{BV}{B'-1} \tag{1}$$

Pressure is obtained by taking volume derivative of the total energy

$$P(V) = \frac{B}{B'}\left[\left(\frac{V}{V_0}\right)^{B'} - 1\right] \tag{2}$$

The bulk modulus pressure derivative

$$B' = \partial B / \partial P \tag{3}$$

The elastic moduli require knowledge of the derivative of the energy as a function of the lattice strain. It is well known that a cubic system has only three independent elastic constants namely C_{11}, C_{12} and C_{44}. Hence, a set of three equations is needed to determine all the constants. The first equation involves calculation of bulk modulus (B), which is related to the elastic constants as:

$$B = \frac{1}{3}(C_{11} + 2C_{12}) \tag{4}$$

The second step involves volume-conservative tetragonal strain given by the following tensor:

$$\begin{bmatrix} \delta & 0 & 0 \\ 0 & \delta & 0 \\ 0 & 0 & \dfrac{1}{(1+\delta)^2} - 1 \end{bmatrix} \tag{5}$$

where $\delta = (1+e)^{-1/3}-1$ with e as strain tensor. Application of this strain has an effect on the total energy from its unstrained value as follows:

$$E(\delta) = E(0) + 3(C_{11} - C_{12}) + V_0\delta^2 + O(\delta^3) \tag{6}$$

where V_0 is the volume of the unit cell.

Finally, for the last type of deformation, we use in the volume-conserving rhombohedra strain tensor given by:

$$\frac{\delta}{3}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \tag{7}$$

which transforms the total energy to

$$E(\delta) = E(0) + \frac{1}{6}(C_{11} + 2C_{12} + 4C_{44}) + V_0\delta^2 + O(\delta^3) \tag{8}$$

The thermal loss mechanisms (temperature dependence) of a material is most suitably described in terms of the Debye temperature (θ_D) which is a fundamental parameter closely related to many physical properties such as elastic constants, specific heat and melting temperature etc. One of the standard methods is to calculate the Debye temperature from elastic constants data, since θ_D may be estimated from the average sound velocity v_m by the following equation [14,15].

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi V_a}\right]^{1/3} v_m \tag{9}$$

where h is Plank's constant, k_B is Boltzmann's constant, V_a is the atomic volume, n is the number of atoms per formula unit and v_m is average sound velocity. The average sound velocity is approximately calculated from [14,16].

$$v_m = \left[\frac{1}{3}\left(\frac{2}{v_t^3}+\frac{1}{v_l^3}\right)\right]^{-1/3} \tag{10}$$

where v_t and v_l are the transverse and longitudinal sound velocities respectively obtained by using the elastic constants as follows:

$$v_l = \sqrt{\frac{\left[C_{11}+\frac{2}{5}(2C_{44}+C_{12}-C_{11})\right]}{\rho}} \tag{11}$$

$$v_t = \sqrt{\frac{\left[C_{44}-\frac{1}{5}(2C_{44}+C_{12}-C_{11})\right]}{\rho}} \tag{12}$$

where C_{11}, C_{12} and C_{44} are second order elastic constants and ρ is mass density per unit volume.

3. Result and discussions

3.1 Structural properties

The total energies are computed in the antiferromagnetic and ferromagnetic states by changing the volume. We have found that ferromagnetic phase is more stable than the antiferromagnetic phase. The magnetic moment of ErCu in the CsCl type structure is calculated to be 2.57 μ_B. The contribution to the total magnetic moment is mainly due to Er '*f*' electrons, while the contribution of Cu atom is negligible. But it is interesting to note that the magnetic moment contributed by Cu atom is negative which indicates that the copper moment is anti-parallel to the RE moment. The equilibrium cell volume of ErCu in the ferromagnetic state is estimated to be 276.63 a.u^3. Therefore in this phase lattice parameter is calculated to be 3.448 Å, which is in good agreement with the experimental value [4]. Our calculated bulk modulus for ErCu is 63.14 Gpa.

3.2 Electronic properties

We have carried out spin-polarized electronic band structure calculations of ErCu and the plotted band structure in majority and minority spin channels shown in Fig 2 and 3, respectively. From these figures one can notice the metallic nature of ErCu. In Fig 2 the bands near -3eV are due to Cu '*d*'- like states. There is a flat band below the Fermi level near -2eV in majority spin due to Er *'f'*- like states which shifts towards the Fermi level near -1eV in minority spin. The Er *'f'*- bands split due to their magnetic behaviour and the other states of both Er and Cu are similar in both spins. We found a value of finite DOS at the Fermi level 0.65states/eV in minority spin which is mainly due Er *'f'* states. We have observed from the DOS and band profile that the 4 *'f'* like states shifted from valence to conduction region due to Er magnetic behaviour, which is dramatic change in metallic behaviour from the Fermi level of ErCu.

Furthermore, the ErCu compound is ductile, because it is consistent with the greater separation between the '*d*' bands and the Fermi level [17].

3.3 Elastic Properties

The elastic constants are important parameters that describe the response to an applied macroscopic stress and especially important as they are related to various solid state phenomena, such as bonding characteristic between adjacent atomic planes, anisotropic factor of binding and structural stability. We have calculated elastic constants of ErCu at ambient pressure by using the method developed by Charpin and integrated it in the WIEN2k package [10]. The calculated values of elastic constants are given in Table. 2 . It can be noted that our calculated elastic constants satisfy the stability criterion: $C_{11} > C_{12}$, $C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{11} > B > C_{12}$ which clearly indicate the stability of the compound in B_2 phase.

3.4 Mechanical Properties

Elastic properties can be used to determine mechanical properties such as Young's modulus (E), shear modulus (G_H), Poisson's ratio (σ) and anisotropic ratio (A) for useful applications. We have calculated these properties of ErCu and presented them in Table 2.

The shear modulus (G_H) describes the material's response to shearing strain using the Voigt-Reuss-Hill (VRH) method [18-20]. The Hill shear modulus (G_H) is given as:

$$G_H = \frac{G_V + G_R}{2} \tag{13}$$

where $G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}$ is the Voigt shear modulus (14)

and $G_R = \frac{5C_{44}(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}$ is the Reuss shear modulus (15)

Using the mechanical and physical properties of these compounds based on their elastic properties, we have analyzed their ductility using the (B/G_H) ratio. The shear modulus (G_H) represents the resistance to plastic deformation while the bulk modulus (B) represents the resistance to fracture. As suggested by Pugh [21], if $B/G_H > 1.75$; a material behaves in a ductile manner. Our B/G_H ratio value is 2.12 indicating the ductile nature of ErCu. Ganeshan *et al.* [22] have established a correlation between the bonding and brittleness/ductility properties. The bond character of cubic compounds is explained with respect to their Cauchy pressure (C_{12} - C_{44}). Compound having more positive Cauchy's pressure tends to form bonds which are primarily metallic in nature, where as the, compounds having more negative Cauchy's pressure from bonds which are more angular or covalent in character [23]. Thus the ductile nature of ErCu can be correlated to their positive cauchy's pressure and thereby metallic character in their bonds.

The Young's modulus (E) is important for technological and engineering application. Young's modulus is defined as the ratio of stress to strain, and is used to provide a measure of the stiffness of the solid, i.e., the larger value of E, the stiffer is the material. It is reported in the literature that stiffer solids have covalent bonds [24]. Young's Modulus (E) is given by-

$$E = \frac{9BG_H}{3B + G_H} \tag{16}$$

It can be seen from the Table 2 that the value of E for ErCu is 79.97GPa . Another important parameter is the elastic anisotropic factor (A), which gives a measure of the anisotropy of the elastic wave velocity in a crystal and it is given as:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \tag{17}$$

which is unity for an isotropic material, anisotropy factor A is listed in Table 2.

The Poisson's ratio (σ) is given by eq (18) as

$$\sigma = \frac{3B - 2G_H}{2(3B + G_H)} \tag{18}$$

It is observed from Table 2 that value of poission's ratio is 0.29.

3.5 Thermal properties

We have calculated the average sound velocities (v_m) and Debye temperatures (θ_D) as well as the density for ErCu phase by using the calculated elastic constants which are given in Table 3.

4. Conclusion

In the present paper, we have investigated the structural and electronic properties of the ErCu. Which crystallizes in CsCl type structure and is stable in ferromagnetic state. The ground state properties like lattice parameters, bulk modulus and magnetic moment are calculated. In addition, we have reported the band structure and density of states of ErCu.In the present study we found $B/G_H > 1.75$ and $C_{12} - C_{44} > 0$; which implies that the ErCu is ductile in nature

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Table 1. Calculated ground state properties, density of states and specific heat for ErCu

Work	Lattice constant a_0 (Å)	Bulk modulus B (GPa)	Pressure derivative B′	Magnetic moment μ_B	Density of states $N(E_F)$ (States/eV)		Specific heat $\gamma = (C_V/T)$ mJ/mole K^2	
					Maj. Spin	Min. Spin	Maj. Spin	Min. Spin
PBE-GGA	3.448	63.14	4.3	2.57	0.65	3.41	1.54	8.04
Exp.	3.430[a]	-	-	-	-	-	-	-

[a]Ref [4].

Table 2. Calculated elastic constant and Young's modulus E, shear modulus G_H, anisotropic factor A, Poisson's ratio σ, Cauchy's pressure C_{12}–C_{44} and B/G_H ratio for ErCu.

Work	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)	E (GPa)	G_H (GPa)	A	σ	C_{12}–C_{44}	B/G_H
ErCu(GGA)	157.23	19.60	16.8	79.97	30.84	0.24	0.29	2.80	2.12

Table 3. Calculated Density, longitudinal ν_l, transverse ν_t, average elastic wave velocities ν_m, Debye Temperature θ_D for ErCu

Work	$\rho*10^3$ (kg/m^3)	ν_l (ms^{-1})	ν_t (ms^{-1})	ν_m (ms^{-1})	θ_D (K)
ErCu (GGA)	7.28	3985	2273	2524	156.71

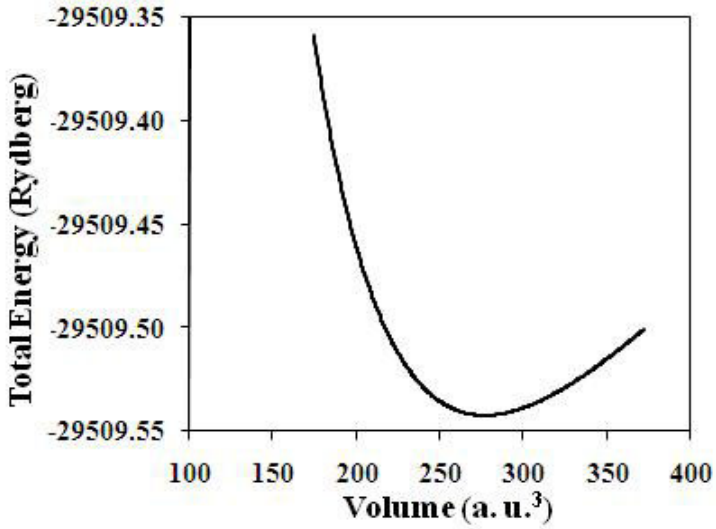

Figure 1. Variation of total energy with volume of ErCu.

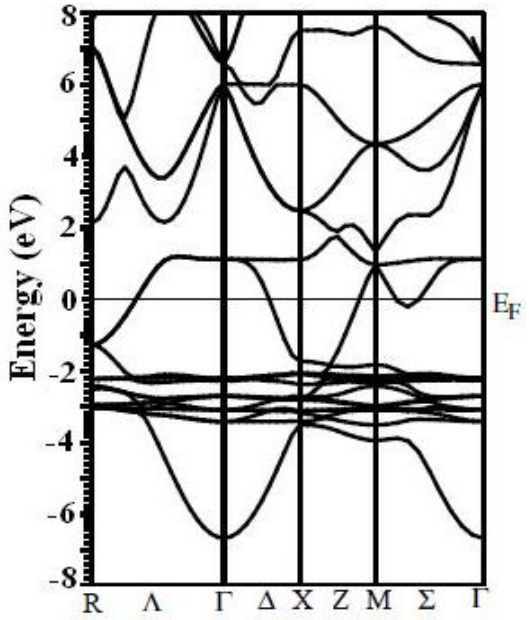

Figure 2. Band structure in majority spin of ErCu.

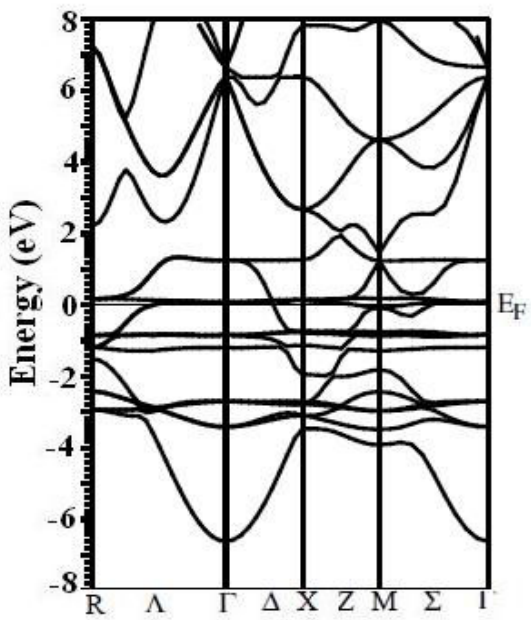

Figure 3. Band structure in minority spin of ErCu

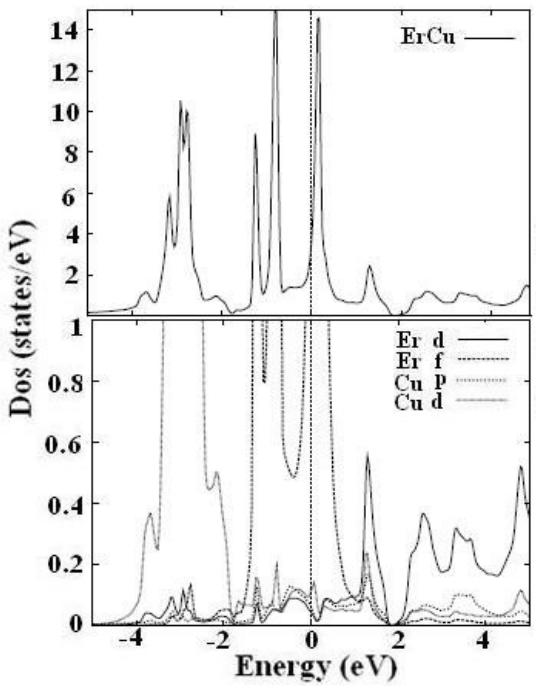

Figure 4. Total and partial density of states in majority spin of ErCu.

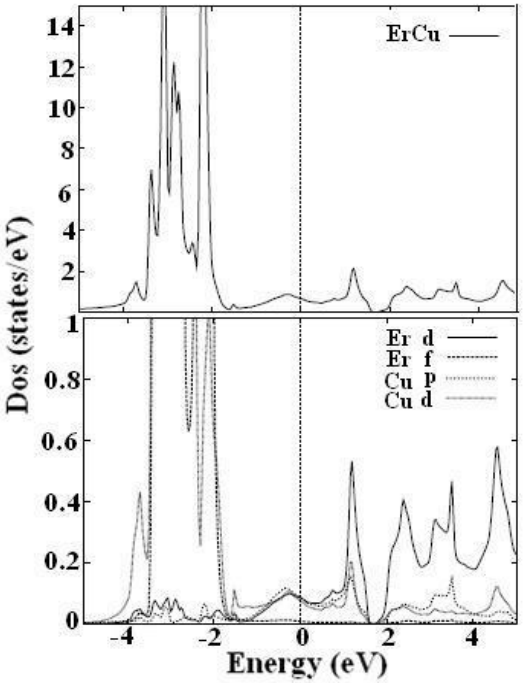

Figure 5. Total and partial density of states in minority spin of ErCu.

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