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Full Potential Linearized Augmented Plane Wave (FP-LAPW) Study of Intermetallic Compound: BeCu

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Abstract *– Electronic structure and elastic properties of berelium based copper intermetallic compound have been investigated in their B_2-type structure (CsCl), Pm3m, space group, 221. The calculations were performed using full potential linearized augmented plane wave (FP-LAPW) method on the basis of density functional theory (DFT). The generalized gradient approximation (GGA) in the scheme of Perdew, Burke and Ernzrhof (PBE) and Perdew et.al. (PBEsol) has been used for the exchange correlation potential. The elastic constants were reported for the first time. From electronic energy band structure (BS) and DOS, the metallic nature of the compound is predicted. The equilibrium properties such as lattice constant (a_0), bulk modulus (B) and its first derivative (B') have also been evaluated. The obtained values of lattice parameter are found to be 2.6941Å and 2.6634Å by PBE-GGA and PBEsol-GGA respectively which are in excellent agreement with experimental data and other theoretical calculations. Similarly the values of reported bulk modulus are 143.29 GPa 157.27 GPa. By the values of calculated elastic constants the mechanical and thermal properties are also predicted.*

Keywords: *FP-LAPW method, intermetallic compounds, band structure, equation of states.*

I. Introduction

The BeCu belongs ‘d’ block transition metal intermetallic compounds. They exists in B_2-type structure (CsCl). Intermetallics are compounds comprised of two or more metals and they are formed when certain combinations of two or more metals are mixed together in certain proportions and react to produce a solid state phase that is distinctively different from the constituent elements. Intermetallics cause’s widespread interests in the scientific research domain, only because of their appealing mechanical properties such as low density, high melting point, good thermal conductivity, and excellent environmental resistance [1-3]. Beryllium copper has long been used for non-sparking tools in the mining, gas and petrochemical industries. Because of the excellent fatigue resistance, beryllium copper is widely used for springs, pressure responsive diaphragms, flexible bellows, connectors, contacts and relays, which all subject to cyclic are loading. *An-ab initio* calculation of the static structural properties of Be have been predicted by Chou et al. [4]. Again Chou et al. [5] presented the structural and electronic properties of beryllium using an *ab-initio* calculation. The calculational method used is the self-consistent Pseudopotential approach within the local-density-functional scheme. Sinko et al. [6] reported the relative Stability and elastic properties of hcp, bcc, and fcc beryllium under pressure using density-functional theory and the full-potential linear-muffin-tin-orbital method. Baranov [7] predicted structural stability of pure elements and binary intermetallic compounds assuming the density of atoms as stationary and un-deformable in internal and external spherical symmetrical shell. Although there is a lot of work carried out on the structural stability, mechanical and other properties of intermetallic compound and their alloys in the literature [1-9]. Rajagopalan et al. [8] reported theoretical lattice parameter and elastic constants of cubic ScX (X = Ag, Cu, Pd, Rh) compounds by performing FP-LAPW study. The structural, electronic and elastic properties of YCu compound was studied by first principles calculations reported by Ugur et al. [9]. Due to the best of authors knowledge there is no systematic reports ever come in light on structural, electronic, mechanical, thermal and elastic behaviour of BeCu intermetallic using FP-LAPW. This motivated us to study of these compounds. The paper is organized as follows. The method of Calculation is briefly described in Section 2. Section 3 deals with the results with discussion of the present work.

II. Method of Calculation

The calculations have been employed by using the full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [10]. It is based upon the density functional theory (DFT) within the generalized gradient approximation (GGA). It is a vibrational method that is presently the most successful approach to compute the electronic structure of matter. The density functional theory is derived from the N-particle Schrödinger equation and useful for systems of very many electrons. For obtaining the results the Perdew, Burke and Ernzrhof (PBE) and Perdew el at. (PBEsol) schemes have been followed for the exchange and correlation effects [11]. Generally the convergence is achieved by expanding the basis function up to $R_{MT}*K_{max}$ = 8.5 for PBE-GGA and 8.0 for PBEsol-GGA, 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 mesh of 1000 k points and the tetrahedral method [12] have been employed for the Brillouin zone integration. The total energies are fitted to Birch equation of state [13] to obtain the ground state properties. 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:

$$B = \frac{1}{3}\left(C_{11} + 2C_{12}\right) \quad (1)$$

One of the standard methods to calculate the Debye temperature is from elastic constants data, since θ_D may be estimated from the average sound velocity v_m by the following equation [14-15]

$$\theta_D = \frac{h}{k_B}\left[\frac{3n}{4\pi V_a}\right]^{\frac{1}{3}} v_m \quad (2)$$

where h is a Planck'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.

III. Results and Discussion

III.1. Structural Properties

For calculating the ground state properties of BeCu, the total energy are calculated as a function of volume in their B_2 (CsCl) phase. The plots of total energy against the reduced volume are shown in Fig. 1. The calculated total energies are fitted to the Birch equation of state [13]. The ground state properties, such as equilibrium lattice constant (a_0), bulk modulus (B) and its first derivative (B') for BeCu have been calculated. The calculated values of these properties are listed in Table 1 and compared with their experimental [16] and other theoretical [7] results. The measured values of lattice constants by both the approximations are in good agreement with the available results or differ in very slight ratio. It is also observed that there is not much difference in our calculated bulk modulus (B) and other theoretical presented bulk modulus.

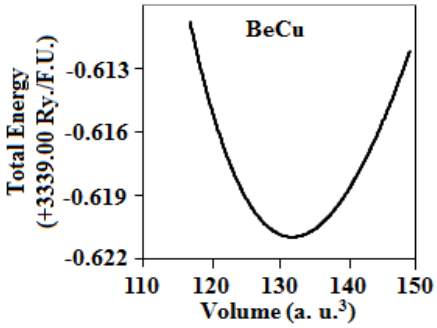

Fig. 1 Variation of total energy with volume for BeCu in B_2 (CsCl - type) structure.

TABLE I
Calculated ground state properties such as lattice parameter (a_0), bulk modulus (B) and its first derivative (B')) for BeCu.

Solid	Work	Approximati-on used	a_0 (Å)	B GPa)	B'
BeCu	Present	PBE-GGA	2.694	143.2	4.31
		PBEsol-GGA	2.663	157.2	4.31
	Exp.	-	2.701[a]	-	-
	Oth. The.	-	2.725[b]	147.8	-

Exp. - Experimental, Oth. The. - Other Theory. [a]Ref. [16], [b]Ref. [7]

III.2. Electronic Properties

The electronic energy band structure for BeCu intermetallic compound along the high-symmetry directions in B_2 phase is obtained using FP-LAPW method within PBE-GGA at ambient pressure, and presented in Fig. 2. The Fermi level E_F is fixed at the origin. It can be seen that there are some bands cross the Fermi level, which indicates the metallic behaviour of BeCu. The total and partial density of states (TDOS and PDOS) is also plotted in Fig. 3. The lowest lying is mainly due to the '*s*' like state of Be nearly -5 eV and do not contribute much to bonding. Many small peaks are observed in the valence bands in the energy range -5 eV to 0 eV only due to '*d*' like states of Cu. The metallicity at the Fermi level is observed due to the joint contribution of four Be '*s*' and Cu '*s*', '*p*' and '*d*' states but there is major participation of '*d*' like state of Cu.
The finite DOS value at Fermi level is obtained as 0.535 states/eV/F.U. which is greater than zero. Hence the compound has obvious metallic character.

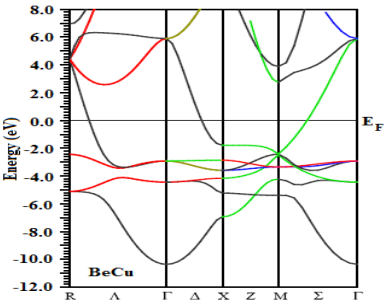

Fig. 2 Electronic Energy Band structure for BeCu.

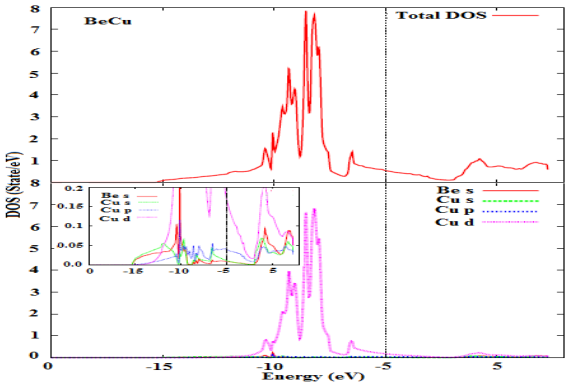

Fig. 3 Density of states for BeCu.

III.3. Elastic Properties

Elastic properties are also associated with sound velocity and Debye temperature. In particular, they provide information on the stability and stiffness of materials. We have calculated the elastic constants for BeCu using PBE-GGA at ambient pressure using the method developed by Thomas Charpin and integrated it in the WIEN2k package [10]. In the present work, the calculated values of second order elastic constants (SOECs) are given in Table 2. It is noticed from Table 2 that our calculated elastic constants satisfy the stability criteria: $C_{11}- C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{12} < B < C_{11}$ and indicate the stability of this compounds in B_2 phase. To the best of Author's knowledge no experimental or theoretical information on the elastic properties of BeCu available in the literature so that they could not be compared.

TABLE II

Calculated elastic properties (value of C_{11}, C_{12} and C_{44}) and density of states at Fermi level $N(E_F)$ for BeCu.

Solid	**Work**	**C_{11} (GPa)**	**C_{12} (GPa)**	**C_{44} (GPa)**	**$N(E_F)$ (States/eV)**
BeCu	PBE-GGA	238.6	99.28	153.2	0.535
	PBEsol-GGA	253.8	111.6	135.7	-

III.4. Mechanical Properties

The elastic constants are essential tool for understanding macroscopic mechanical properties of crystal as they relate to various fundamental solid state properties and thermodynamic properties. The mechanical properties such as Young's modulus (E), Shear modulus (G_H), Poisson's ratio (ρ), anisotropic ratio (A), are calculated for useful applications and their values are inserted in Table 3. The shear modulus G_H describes the material's response to shearing strain using the Voigt-Reuss-Hill (VRH) method [17-19]. The effective modulus for the polycrystals could be approximated by the arithmetic mean of the two well known bounds for mono crystals. The Hill shear modulus G_H is given as:

$$G_H = \frac{G_V + G_R}{2} \tag{3}$$

where $G_V = \frac{C_{11} - C_{12} + 3C_{44}}{5}$ is the Voigt shear modulus. (4)

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

Using the mechanical and physical properties of these compounds based on their elastic properties, we have analyzed their brittleness 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 [20], if $B/G_H > 1.75$; a material behaves in a ductile manner otherwise brittle nature. The (B/G_H) ratio for BeCu is found to be 1.30, indicating its brittle nature. Ganesham et al. [21] has established a correlation between the binding properties and ductility. The bond character of cubic compounds is explained with respect to their Cauchy pressure (C_{12}–C_{44}). Compounds having more positive Cauchy pressure tend to form bonds which are primarily metallic in nature, where as compounds having more negative Cauchy pressure form bonds which are more angular in character [22]. Thus, the brittle nature of BeCu compound, can be correlated to their negative Cauchy pressure and thereby the more angular in 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 and 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. And the stiffer solids have covalent bonds [23]. Young's Modulus E is given by

$$E = \frac{9BG_H}{3B + G_H} \tag{6}$$

It can be seen from Table 3 that BeCu have higher value of E implying to be more covalent in nature. The Poisson's ratio (r) is given by Eq. (7) as

$$\sigma = \frac{3B - 2G_H}{2(3B + G_H)} \quad (7)$$

It is observed from Table 3 that value of Poisson's ratio for BeCu is 0.194. 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:

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \quad (8)$$

For an ideal isotropic system, *A* is unity and deviation from unity measures the amount to elastic anisotropy. The calculated anisotropy factor for BeCu greater than 1 which shows that these compounds are elastically anisotropic.

TABLE III

Calculated anisotropy factor (*A*), Shear modulus (G_H), Young's modulus (*E*), Poisson's ratio (σ), (B/G_H) ratio and Cauchy's pressure (C_{12} - C_{44}) for BeCu using PBE-GGA.

Solid	**A**	**G_H (GPa)**	**E (GPa)**	**σ**	**B/G_H**	**C_{12} - C_{44} (GPa)**
BeCu	2.20	111.8	267.1	0.19	1.30	-54.30

III.5. Thermal Properties

To get the knowledge of many fundamental solid state properties such as specific heat, stability of lattice, melting point and so on, the Debye temperature is the easiest parameter ever used. By putting the values of calculated elastic constants, the thermal properties of the material in B_2-phase can be determined and inserted in Table 4. In the absence of any measured data, they could not be compared. Hence, our results will help in the future prediction for these properties of BeCu intermetallic compound.

TABLE IV

Calculated density (ρ), longitudinal (v_l), transverse (v_t), average elastic wave velocities (v_m) and Debye temperature (θ_D) for BeCu using PBE-GGA.

Solid	**ρ x 10^3 (kg/m^3)**	**v_l (m/s)**	**v_t (m/s)**	**v_m (m/s)**	**θ_D (K°)**
BeCu	24.722	3516.83	2203.36	2424.76	332.7

IV. Conclusion

We have studied the structural, electronic, thermal and elastic properties of BeCu intermetallic compound using FP-LAPW method based on density functional theory in the B_2 structure. The total energy is fitted to the Birch equation of state. The obtained lattice constants are in good agreement with the available experimental and other theoretical values. The ground state properties like bulk modulus and its first derivative are also calculated. We have plotted electronic band structure and DOS for BeCu in the B_2 phase by using PBE-GGA approximation which shows that BeCu is metallic in nature. The calculated elastic constants justifies that BeCu compound is elastically stable in the B_2 phase. Using the values of these elastic constants, the shear modulus (*G*), Young's modulus (*E*), Poisson's ratio (σ) and anisotropic ratio (*A*) are also reported.

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