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Density Functional Calculations on Structural and Elastic Properties of BeCo Intermetallic under Pressure

Ekta Jain[1], Gitanjali Pagare[1*] and Sankar P. Sanyal[2]

[1]Department of Physics, Government M. L. B. Girls P. G. Autonomous College, Bhopal 462002, India

[2]Department of Physics, Barkatullah University, Bhopal 462026, India

Abstract

The structural and elastic properties of beryllium cobalt intermetallic compound in B_2-type (CsCl) structure are studied. The calculations were performed employing full potential linearized augmented plane wave (FP-LAPW) method. It is based on density functional theory (DFT). The generalized gradient approximation (GGA) in the scheme of Perdew, Burke and Ernzrhof (PBE) Wu and Cohen (WC) and Perdew et al. (PBE-sol) has been used for the exchange correlation potential. The equilibrium properties such as lattice constant (a_0), bulk modulus (B) and its first derivative (B') have been obtained. The calculated equilibrium lattice parameters are in excellent agreement with the available experimental and other theoretical results. We first time report the variation of elastic constants under pressure range (0 GPa - 20 GPa).

Keywords: FP-LAPW method, intermetallic compounds, elastic constants, equation of states.

4. Introduction

The BeCo belongs to 'd' block transition metal intermetallic compound family. It exists in B_2-type (CsCl) crystal structure. 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]. In recent years, the significant advances in computational materials science have made possible the use of *ab-initio* quantum mechanical techniques to predict structural, electronic, thermal and elastic properties of the compounds and their alloys. By employing the self consistent ultra soft pseudopotential method Ugur et al. [4] reported the structural, electronic and vibrational properties of ordered intermetallic alloys CoZ (Z = Al, Be, Sc and Zr). Cheng et al. [5] presented the first principles study of elastic properties and electronic structure of NiTi, CoTi and FeTi. *An-ab initio* calculation of the static structural properties of Be have been predicted by Chou et al. [6]. Again Chou et al. [7] 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. Baranov [8] 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, electronic, elastic, thermal and other properties of intermetallic compound and their alloys in the literature [1-8]. Due to the best of authors knowledge there is no systematic reports ever come in light on structural and elastic behaviour of BeCo intermetallic using FP-LAPW under pressure. This motivated us to study of this compound. 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.

5. Computational Method.

The calculations have been performed using the full potential linearized augmented plane wave (FP-LAPW) method as implemented in the WIEN2k code [9]. 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), Wu and Cohen (WC) and Perdew et al. schemes has been followed for the exchange and correlation effects [10]. Generally the convergence is achieved by expanding 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 $G_{max} = 12$ $(Ryd)^{1/2}$. 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 [11] have been employed for the Brillouin zone integration. The total energies are fitted to Birch equation of state [12] 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:

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

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

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

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

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

where V_0 is the volume of the unit cell.

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

$$\frac{\delta}{3}\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix} \tag{4}$$

which transforms the total energy to

$$E(\delta) = E(0) + \frac{1}{6}(C_{11} + 2C_{12} + 4C_{44}) + V_0\delta^2 + 0(\delta^2) \tag{5}$$

6. Result and discussion

6.1. Ground state properties

In order to calculate the ground state properties of Beryllium cobalt, the total energy are calculated as a function of reduced volume in their and B_2-type (CsCl) structure using full potential linearized augmented plane wave (FP-LAPW) method. 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 [12] to investigate the volume-energy relationship. The ground state properties, such as equilibrium lattice constant (a_0), bulk modulus (B) and its first derivative (B') for BeCo have been calculated in their B_2-phase by all the GGA approximations mentioned. The calculated values of these properties are tabulated in Table 1 and compared with their experimental [13] and other theoretical [8] results. On the inspection of Table 1 we found that the measured value of lattice constants using PBE-GGA are found to be in close agreement with the available experimental and previous theoretical values than other GGA calculations. It is also observed that our calculated bulk modulus (B) overestimates the other theoretical data for the same which may be due to the different approximations used in the calculation. The variation of volume with pressure is also studied for this compound in CsCl structure and presented in Fig. 2 by all the approximations used. It is observed that the cell volume decreases with increasing pressure.

6.2. *Elastic properties:*

The elastic constants are fundamental and indispensable for describing the mechanical properties of materials. There are 21 independent elastic constants, but the symmetry of cubic crystal reduces this number to

only three independent elastic constants i. e. C_{11}, C_{12} and C_{44}. The bulk modulus B for cubic systems is expressed as a linear combination of C_{11} and C_{12}. We have calculated the elastic constants for BeCo using PBE-GGA, WC-GGA and PBE-sol GGA approximations at ambient pressure employing the method developed by Thomas Charpin and integrated it in the WIEN2k package [9]. The calculated values of elastic constants are also listed in Table 1. It can be noticed that our calculated elastic constants satisfy the stability criterions: $C_{11} - C_{12} > 0$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$, $C_{12} < B < C_{11}$, which clearly indicate BeCo intermetallic compound is stable in B_2-type (CsCl) crystal structure. For BeCo, to notice the effect of pressure on the elastic constants, the pressure dependence behaviour of the second-order elastic constants is also investigated up to 20 GPa shown in Fig 3. It is found that all the three elastic constants (C_{11}, C_{12} and C_{44}) increase linearly with the variation in the pressure.

Conclusion

We have performed the *ab-initio* calculations to evaluate the structural and elastic properties of BeCo binary intermetallic compound with B_2-type (CsCl) structure using full potential linear augmented plane wave method (FP-LAPW) on the basis of density functional theory (DFT). We have applied the three schemes of generalized gradient approximations (PBE-GGA, WC-GGA and PBEsol-GGA) for the calculations. The total energy is fitted to the Birch equation of state. The ground state properties like lattice parameter, bulk modulus and its pressure derivative are calculated. The obtained lattice constants are in good agreement with the available experimental and theoretical values. The second order elastic constants at ambient and high pressure are reported, which satisfy the mechanical stability criterion.

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Table 1

The calculated ground state properties and elastic properties for BeCo at ambient pressure.

Solid	Work	Approx.	a_o (Å)	B (GPa)	B'	C_{11} (GPa)	C_{12} (GPa)	C_{44} (GPa)
BeCo	Present	PBE-GGA	2.5912	199.84	3.98	322.78	142.43	166.75
		WC-GGA	2.5680	213.28	3.93	359.13	143.14	176.21
		PBEsol-GGA	2.5647	219.00	4.29	362.75	143.98	172.30
	Exp.	-	2.611[a]	-	-	-	-	-
	Oth. The.	-	2.712[b]	177.79[b]	-	-	-	-

Exp. - Experimental, Oth. The. - Other Theory, Approx. – Approximations

[a]Ref [13]

[b]Ref [8]

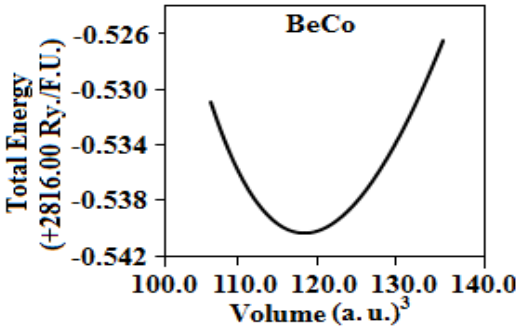

Fig.1 Variation of total energy with volume

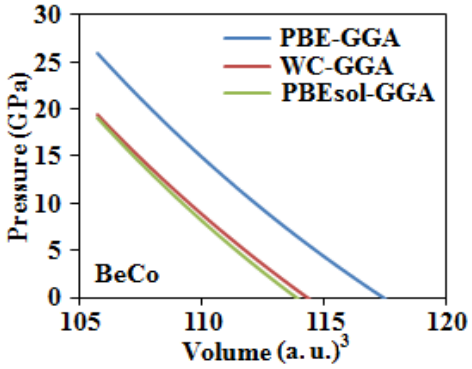

Fig.2 Variation of pressure with volume

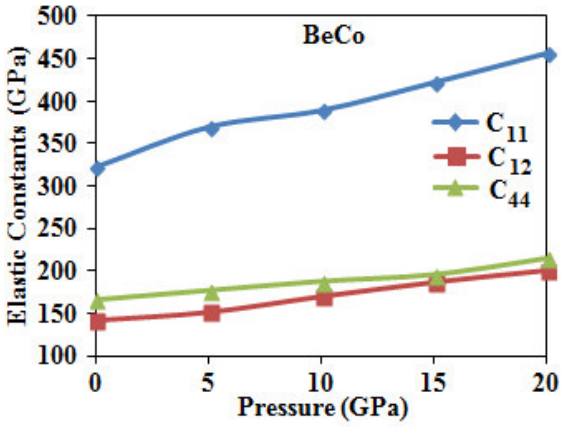

Fig.3 Variation of Elastic Constants with Pressure

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