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Masood Ayoub Kaloo *

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Research Article

Computational Study of the Structural, Elastic and Mechanical Properties of Cobalt Alloys

Tajamul Islam [1], Rafeeq Ahmed Mir [2], Bial A Bhat [3] and Masood Ayoub Kaloo [4*]

[1] Department of Physics, Govt. Degree College Shopian-192303 J&K, India.

[2] School of Studies in Physics, Jiwaji University Gwalior-474011 M.P, India.

[3] Department of Chemistrys, Govt. Degree College Shopian-192303 J&K, India.

[4] Department of Chemistry, Govt. Degree College Doda-182202 J&K, India.

***Corresponding Author:** Masood Ayoub Kaloo, Department of Physics, Govt. Degree College Shopian-192303 J&K, India.

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Abstract

In this present work, bonding, crystal structure, electronic and charge density like properties of cobalt alloys (CoNi and CoFe) were investigated theoretically with the help of computational calculations like density functional theory (DFT) and time-dependent density functional theory (TD-DFT). The computation performed with full-potential linearized augmented plane wave (FPLAPW) and embedded in Wien2k using different basis sets showed that the ferromagnetic (FM) cubic structure is energetically the most stable state for both these alloys. The given alloys were found to be stiffer because of stronger bonding in them. Their valence and conduction bands were also found to be overlapped, indicating metallic-like behaviour.

Key words: bonding; crystal; DFT; ferromagnetic; metallic

Introduction

Among various materials, bimetallic alloys have deciphered immense importance with diverse scopes in various fields. However it is only Fe, Co, Ni and their alloys (CoFe, CoNi and FeNi) which display ferromagnetic performance at room temperature [1]. Owing to their unique physical and chemical characteristics like high permeability, high Curie temperature, low coercivity, less dielectric constant, high chemical robustness and mechanical hardness, CoFe and CoNi alloys encompass high scope in day to day life [2]. They have as well attracted much attention of researchers because of their importance in future magnetic device applications such as magnetic tunnel junctions [3]. Because of their soft magnetic behaviour with high saturation magnetization along with high Curie temperatures, their nanoparticles have been widely studied experimentally for different applications [5-9]. Keeping in view such diverse applications, computational calculations have been utilized to understand numerous physical and chemical properties like elastic compliance constants or simply elastic constants (ECs) [10-13]. With the help of ECs, various physical properties like melting temperature, bulk modulus, hardness, Voigt's modulus, Hill's modulus, shear modulus, Reuss's modulus, Young's modulus, Poisson's ratio, and elastic stiffness coefficients have been calculated [14]. The core properties like band structure, density of states and transport properties can be obtained with well-established computational tools.

Currently, commercially available thermo electric (TE) materials are rare, expensive and toxic but it is an urgent need to develop new, cheap, abundant and environment-friendly alternatives. Thus it is important to study computational calculation and other theoretical basics so as to have better understanding of their properties, modifications and hence their diverse futuristic applications.

Methods of Computation

Regarding the prediction and explanation of physical properties, and other important characteristics, DFT is highly important along with FPLAPW method embedded in Wien2k [15].

Results and Discussion

Structural properties

The structural properties are highly significant for understanding of the various material properties so as to deduce the valuable information about the nature of bonding and diverse interactions. According to the literature, CoFe and CoNi compounds crystallise in cubic B2 structure with *Pm-3m* (221) space group. Here Co atom occupies the (0.0, 0.0, 0.0) Wyckoff positions whereas Fe or Ni atoms occupy the (0.5, 0.5, 0.5) site. In order to determine ground state properties for both FM and non-magnetic (NM)

states, volume optimization is carried out. In both FM and NM phases, the variation of total energy *w.r.t* volume is represented by Fig. 1 for CoFe and CoNi intermetallics. The computational calculations showed that the ferromagnetic structure is energetically the most stable state for both the alloys. Therefore, we have investigated the ground state properties and thermoelectric properties of CoX (Fe, Ni) binary alloys. The optimised value of lattice parameters are found to be a_0 = 2.845 Å for CoFe and a_0 = 2.830 Å for CoNi using the first-principles FP-LAPW method.

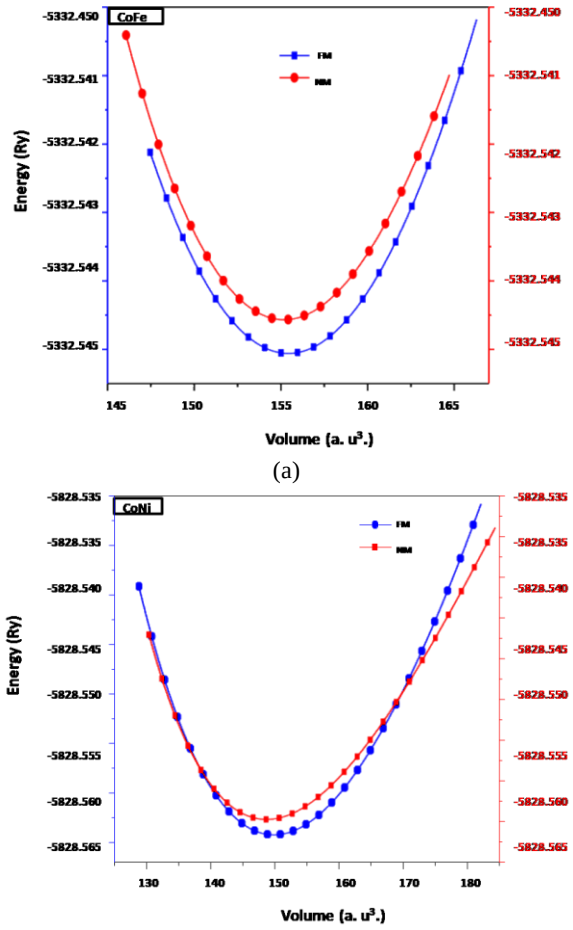

Figure. 1: Total energy versus Volume for CoFe (a), and (b) CoNi alloys.

1.Elastic (E) and Mechanical (M) Properties

E and M properties play an imperative part to know the valuable information about the bonding characteristic between adjacent atomic planes, anisotropic character and structural stability. The elastic constants of CoFe and CoNi intermetallics at ambient pressure were calculated by using the method (Charpin) and integrated with WIEN2k package. The EC's along with bulk modulus (B) and shear modulus calculated *via* Voight–Reuss–Hill (VRH) approximation are given in Table 1. It can be noted that our calculated elastic constants satisfy the stability criteria [18]; $C11 - C12 > 0$, $C11 > 0$, $C44 > 0$, $C11 + 2C12 > 0$ and $C12 < B < C11$ which clearly indicate the stability of these compounds in B2 phase. The hard nature of CoFe and CoNi alloys could be understood in terms of their high bulk modulus. Since Bulk modulus (B) and shear modulus (GH) also measure the resistance of the material to volume and shape change, hence our results indicate that both CoFe and CoNi are more inclined to resist with volume change than shape change. It indicates that both the alloys are stiffer and hence, are suggestive of strong bonding.

Alloy	C11	C12	C44	B	GV	GR	GH
CoFe	316.53	139.76	184.86	198.68	146.27	128.67	137.47
CoNi	305.14	130.58	163.76	188.76	133.16	121.25	127.20

Table 1: Elastic constants (C11, C12 and C44), Bulk modulus (B), Voigt's Shear (GV) modulii, Reuss's Shear (GR) moduli and Shear modulus (GH) in GPa.

Conclusion

In this presents work, the various physical properties of alloys of cobalt were investigated theoretically with the help of DFT and TD-DFT. The computation performed indicated that the ferromagnetic cubic structure of both alloys is energetically the most stable state. They were also found stiffer indicating

strong bonding in them. The valence and conduction bands were found overlapped, reflecting their metallic character.

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