Review Article

Electronic and Magnetic Properties of GdNiBi Compound Using DFT

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Abstract

The electronic and magnetic properties of GdNiBi ternary rare earth compounds were examined using the WIEN 2K simulation software. The compound in question exhibits semiconductor characteristics, as evidenced by its electronic properties, which indicate a band gap of 0.2 eV. The magnetic properties of the material indicate an antiferromagnetic nature, with a Néel temperature (T_N) that is lower than 16 Kelvin. The temperature at which a material undergoes a transition is heavily influenced by the conditions under which it is prepared. The electronic band structure calculations are in concurrence with both the magnetic and electronic behaviour.

Keywords: DFT, Magnetic Properties, WIEN2K, Rare Earth Compound.

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Introduction

For a considerable period, solid-state chemists and physicists have been engaged in the endeavour of improving the properties of materials, such as their thermoelectric, magnetic, and piezoelectric characteristics. In order to enhance comprehension of electronic characteristics, it is imperative to conduct a comparative analysis of empirical and theoretical findings. The present study offers theoretical findings regarding the ternary rare earth compound GdNiBi. Ternary rare earth compounds' magnetic and electronic characteristics RETX have been the focus of a lot of recent studies (where RE stands for rare earth, T is for transition metal, and X is for a p- block element). The system provides a broad range of structural options [1, 2]. This family exhibits a particular interest in compounds possessing 18 valence electrons and featuring the MgAgAs structure type (C1b structure, F4¯3m). The compound in question has been demonstrated to possess characteristics of a closed shell species, exhibiting non-magnetic and semiconducting properties, or alternatively, a pseudo-gap at Fermi energy, as evidenced by sources [3, 4]. The localization of f-electrons in rare earth metals precludes their classification as valence electrons. While GdNiBi has been recognised for a certain period of time [5-7], additional studies pertaining to its magnetic and electronic properties have only been conducted for the GdNiSb compound [8–11]. One noteworthy characteristic of certain GdNiSb compounds is their ability to exhibit semiconductor properties despite being comprised solely of metallic elements. A recent study [12] investigated the genesis of gap formation in this compound. Due to its isoelectric nature, GdNiBi exhibits certain properties. Spin-polarized electronic band structure calculations were conducted in order to comprehend the relationship between structure and properties. The study employed the FLAPW method in conjunction with the GGA scheme, as outlined in reference[13]. The findings were juxtaposed with electronic and magnetic assessments.

Computational Method

The calculations' approach is based on the density functional theory (DFT)-based full-potential linearized augmented plane wave (FP-LAPW) technique [13–15]. In WIEN2K, this strategy has been used. The generalised gradient approximation (GGA) method developed by Perdew, Burke, and Ernzerhof (PBE) was used to optimise the structure. The calculations pertaining to electronics and magnetism were conducted utilizing the Generalized Gradient Approximation (GGA) method [16]. To achieve accurate energy convergence, the RMTKmax parameter was established at a value of 7. In this case, Kmax denotes the largest possible size of the k vector in the plane wave expansion, while RMT stands for the atomic radius inside the unit cell. The unit cell is split into two separate sections, the atomic spheres and the interstitial region, as part of the FP-LAPW approach. While in the interstitial region these wave functions are extended using a plane wave basis, they are extended within the atomic sphere region using atomic-like functions. Lmax, the symbol for the greatest amount of angular momentum, was given the number 10. The value of Gmax was also determined to be 12 atomic units per negative one. The achievement of a condition in which the total energy displays stability within a margin of 0.001 Ry and the charge discrepancy is below 0.001 e/a.u.3 per unit cell is the definition of the energy and charge convergence criterion in the current inquiry. Using a mesh made up of 1500 K points and the tetrahedral technique, the Brillouin zone integration was completed [17].

Results and Discussion

Structural properties

As seen in Figure 1, the cubic MgAgAs (C1b structure, F4 3m) structure type of GdNiBi's crystal structure is what distinguishes it from other crystal structures. In Table 1, the GdNiBi compounds' lattice characteristics. The findings are consistent with prior research [6, 7]. The

magnesium sites in the compounds $RE^{3+}NiBi^{3-}$ include trivalent cations with electropositive characteristics. The configuration can be characterized as a MgAs-filled NaCl structure, wherein Ni atoms are incorporated into 50% of the tetrahedral voids (Ag sites). The compound under consideration can be interpreted in two ways: either as Ni atoms situated as a filled ZnS zincblende type structure or within the host $RE^{3+}Bi^{3-}$ structure $NiBi^{3-}$, wherein the octahedral holes are occupied by RE^{3+} atoms. Excluding comparable permutations, this structure with a face-centered cubic arrangement exhibits three distinct potential atomic distributions. Thereby resulting in narrower bands and the possibility of gaps in the density-of-states (DOS) spectrum [12].

Table-1

Compound	Space Group	Lattice parameter(Å)	Gd	Ni	Bi
GdNiBi	$F\bar{4}3m$ (216)	$a_0=b_0=c_0=$ 6.600	(0.5, 0.5, 0.5)	(0.25, 0.25, 0.25)	(0, 0, 0)

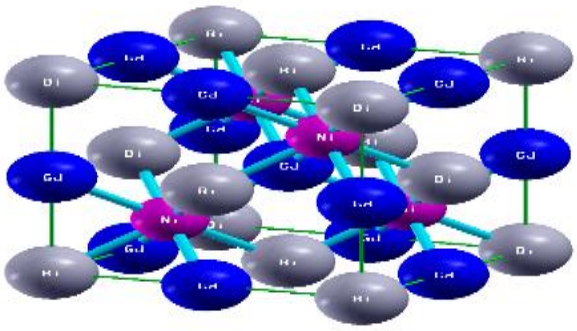


Fig-1 GdNiBi crystal structure generating XCrySDen software.

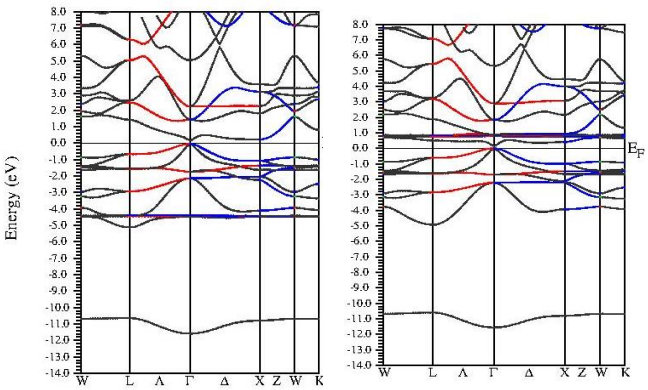
Electronic properties

he FLAPW method [12] was employed for band structure calculations using the self-consistent approach, as depicted in Figure 2. The PBE-GGA implementation of the Perdew-Burke-Ernzerhof method was utilized to conduct the calculations [15]. A value of 2.5 Bohr was employed as the muffin-tin radius (RMT) for each individual atom. The employed calculations were self-consistent and utilized a grid consisting of no less than 24 x 24 x 17 k points located within the primitive wedge of the Brillouin zone [18]. Figure 2 depicts the band structure calculation for both spin up and spin down. The figure illustrates that the majority of the band is situated within the range of -5.0 eV to 0.0 eV for both the spin-up and spin-down channels. The semiconductor nature of the GdNiBi compound is evidenced by the presence of a forbidden gap between its valence and conduction bands, as per the band structure analysis. The origin of this structure is primarily attributed to the Ni 3d orbitals. A minor contribution is derived solely from the occupied Bi 5s 5p orbitals. The band gap is estimated to be around 0.2 electron volts.

Magnetic properties

The magnetic characteristics of a material can be described in relation to its magnetic moment. Table 2 displays the magnetic moment. The spin magnetic moment is attributed to the Gd-f state.

S.No	compound	Spin Magnetic Moment Value in μB
1.	Interstitial region	0.13047
2.	Gd	6.95642
3.	Ni	-0.05731
4.	Bi	-0.02951
5.	Total (GdNiBi)	7.00007



Spin Up **Spin Down**

Fig-2 Band structure for GdNIBi Compound

Conclusion

In brief, the electronic characteristics and magnetic attributes of GdNiBi compounds were expounded. The GdNiBi compound exhibits antiferromagnetic behaviour at low temperatures. The antiferromagnetic ground state of this compound has been confirmed through GGA approximation calculations. Moreover, the GGA approximation computations exhibit complete concurrence with the electronic measurements.

The compound GdNiBi exhibits semiconducting properties.

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Conflict of interest: Nil
Acknowledgement: None

References

[1] R.-D. Hoffmann, R. Pöttgen, Z. Kristal logr., 216, 127, (2001).
[2] R. Pöttgen, D. Johrendt, Chem. Mater.12, 875, (2000).
[3] H. C. Kandpal, R. Seshadri, C. Felser, J. Phys. D: Appl. Phys. 39, 776, (2006).
[4] J. Köhler, S. Deng, C. Lee, M.-H. Whangbo, Inorg. Chem. 46, 1957, (2007)
[5] A. E. Dwight, J. Less-Common Met. 34, 279, (1974).
[6] A. E. Dwight, in: Proceedings of Rare Earth Research Conference 11th, J. M. Haschke, H. A. Eick (eds), NTIS, Springfield, VA, 642, (1974).
[7] M. G. Haase, T. Schmidt, C. G. Richter, H. Block, W. Jeitschko, J. Solid State Chem.168, 18, (2002).
[8] H. Hartjes, W. Jeitschko, J. Alloys Compds. 226, 81, (1995).
[9] R. V. Skolozdra, A. Guizik, A. M. Goryn, J. Pierre, Acta Phys. Pol. A 92, 343, (1997).
[10] I. Karla, J. Pierre, R. V. Skolozdra, J. Alloys Compds. 265, 42, (1998).
[11] I. Karla, J. Pierre, B. Ouladdiaf, Physica B. 253, 215, (1998).
[12] P. Larson, S. D. Mahanti, S. Sportouch, M. G. Kanatzidis, Phys. Rev. B 59, 15660, (1999).
[13] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, J. Lu- itz, WIEN2k, An Augmented Plane Wave + Local Orbitals Program for Calculating Crystal Properties, 2001.
[14] Z. Wu, R.E. Cohen, Phys. Rev. B 73 (2006).
[15] J. P. Perdew, K. Burke, M. Enzerhof, Phys. Rev. Lett. 77, 3865, (1996).
[16] F. Tran, P. Blaha, Phys. Rev. Lett. 102, 226401, (2009).
[17] H.J. Monkhorst, J.D. Pack, Phys. Rev. B 13, 5188, (1976).
[18] W. Haberditzl, Magnetochemie, Akademie-Verlag, Berlin, (1968).

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