A DFT-Based Comparative Study on the Structural, Magnetic, Electronic, and Thermoelectric Properties of $TMCo_2$ (TM = Ti, Nb) Intermetallics

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Abstract

In this work, we present a comparative study of the structural, magnetic, electronic, and thermoelectric properties of cubic binary Laves-phase intermetallic compounds with the general formula $TMCo_2$ (TM = Ti, Nb), using density functional theory (DFT) within the Wien2k code. Geometrical optimization, performed through the Birch-Murnaghan equation of state, shows excellent agreement with prior theoretical and experimental findings. The magnetic properties confirm the presence of ferromagnetic ordering. To explore the electronic properties, we have analyzed the band structures and density of states.

Keywords: Lave Phase; Bulk Modulus; Birch Murnaghan Equation.
Received 30 January 2025; First Review 10 February 2025; Accepted 16 February 2025

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How to cite this article
Hansraj Dhadse, Suparn Kumar Barmase, Shubha Dubey, Jagdeesh Pataiya, and Chandrabhan Makode, A DFT-Based Comparative Study on the Structural, Magnetic, Electronic, and Thermoelectric Properties of $TMCo_2$ (TM = Ti, Nb) Intermetallics, J. Cond. Matt. 2024; 02 (02): 53-55

Available from:
https://doi.org/10.61343/jcm.v2i02.106

Introduction

The Laves phase, found in over 900 systems, is an intermetallic compound known for properties like wear resistance, hardness, and superconductivity, which depend on its chemical composition [1]. Laves phases hold great potential for various applications. For example, $TiCo_2$ compounds have been employed as hydrogen storage materials due to their excellent hydrogen absorption capabilities and favorable hydriding-dehydriding kinetics [2]. Additionally, (Tb, Dy)Fe_2 and (Al, Fe)Zr_2 have been explored for magnetoelastic transducer applications owing to their remarkable magnetostriction. $TiCo_2$ and $NbCo_2$ alloys exhibit superconducting properties, including high critical temperatures, strong magnetic fields, and high current densities [3]. Furthermore, $NbCo_2$ and $TiCo_2$-based two-phase alloys are well-suited for high-temperature structural applications, thanks to their high melting points and exceptional retention of mechanical properties at elevated temperatures. In this paper, we have investigated the structural and electronic properties of $TMCo_2$ (TM = Ti and Nb) Laves phase compounds.

Computational Method

For DFT-based ground-state energy calculations, the Wien2k software is used in conjunction with the FP-LAPW approach [4]. PBE-GGA describes the exchange-correlation potential, while RMTKmax, the energy convergence parameter, is set to 7.0. Self-consistency is attained when the total energy stabilises within 10^{-4} Ry, with the Gmax parameter set to 12 a.u.$^{-1}$. The Brillouin zone integration is performed using the Monkhorst-Pack method with 1000 k-points, and the valence and core states are separated using a cut-off energy of -6.0 Ry with a charge convergence threshold of 0.0001e.

Results and Discussions

The $TMCo_2$ (TM = Ti and Nb) compounds crystallize in the cubic Laves phase structure, belonging to the $Fd\bar{3}m$ space group (No. 227). This structure is characterized by a densely packed arrangement of atoms, where TM and Co atoms occupy specific Wyckoff positions, forming a three-dimensional framework with high symmetry.

Table 1: Optimized structural parameters

Parameters	$TiCo_2$	$NbCo_2$
a (Å)	7.0997	7.4001
V (Å^3)	603.76	683.0782
B (GPa)	93.7626	132.2316
B´	5.0676	4.7633
E_0	-12404.149032	-36137.279837

The structural properties of $TiCo_2$ and $NbCo_2$ compounds satisfy the Birch-Murnaghan equation of state, and both compounds exhibit ferromagnetic behavior. The Birch-Murnaghan equation of state is used to describe the pressure-volume relationship, confirming the stability of the cubic $Fd\bar{3}m$ structure for $TiCo_2$ and $NbCo_2$. Additionally, both compounds are ferromagnetic in nature, characterized by a net magnetic moment arising from the alignment of magnetic moments in the same direction. This makes them promising candidates for applications in magnetic and spintronic devices. The ferromagnetic energy versus volume curve for both $TiCo_2$ and $NbCo_2$ compounds is presented in Figure 1. The optimized structural parameters obtained from the calculations align well with previously reported experimental results [5], confirming the reliability of the computational approach used in this study.

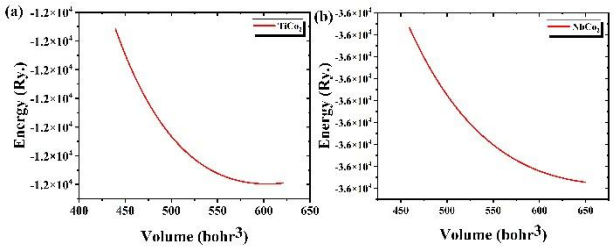

Figure 1: Energy Versus volume curve for $TMCo_2$ (TM= Ti and Nb).

The magnetic properties of $TiCo_2$ and $NbCo_2$ Laves phase compounds reveal distinct behaviors. In $TiCo_2$, the transition metal (Ti) contributes a small magnetic moment of $0.03134\mu_B$, while the cobalt atoms provide the dominant contribution with a magnetic moment of $0.50612\mu_B$. The interstitial regions exhibit a slight negative moment of $-0.06847\mu_B$, leading to a total magnetic moment of $1.06913\mu_B$ for the unit cell, confirming its ferromagnetic nature. Conversely, $NbCo_2$ displays negligible magnetism, with the transition metal (Nb) contributing $-0.00002\mu_B$ and cobalt only $0.00012\mu_B$. The interstitial contribution is nearly zero at $-0.00001\mu_B$, resulting in a total magnetic moment of $0.00015\mu_B$, indicating that $NbCo_2$ is essentially non-magnetic. This highlights the stark contrast in magnetic properties between the two compounds. The spin-polarized density of states (DOS) for $TiCo_2$ and $NbCo_2$ Laves phase compounds, as shown in Figure 2, highlights their metallic and ferromagnetic nature. The total DOS for both compounds exhibit significant spin polarization, with an asymmetry between the spin-up and spin-down states, confirming their ferromagnetic behaviour. The Co atoms contribute dominantly to the DOS near the Fermi level (E_f) due to their partially filled d-orbitals, while the transition metals (Ti in $TiCo_2$ and Nb in $NbCo_2$) also contribute through hybridization with Co d-states. The position of E_f within regions of finite DOS for both spin channels further confirms their metallic behaviour. This interplay of electronic and magnetic properties makes $TiCo_2$ and $NbCo_2$ promising candidates for applications in spintronic and magnetic devices.

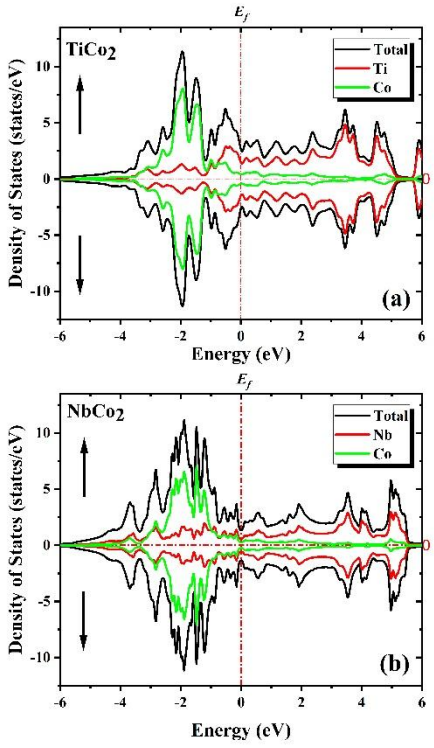

Figure 2: Electron Density of States of $TiCo_2$ and $NbCo_2$

Conclusion

In conclusion, the $TiCo_2$ and $NbCo_2$ compounds, both crystallizing in the cubic Laves phase structure, exhibit distinct magnetic behaviors. $TiCo_2$ shows ferromagnetism with a total magnetic moment of $1.06913\mu_B$, while $NbCo_2$ is nearly non-magnetic. Both compounds are metallic with significant spin polarization, primarily driven by cobalt atoms. The computational results align well with experimental data, confirming the stability and ferromagnetic nature of $TiCo_2$. These compounds show

promising potential for applications in magnetic and spintronic devices due to their unique electronic and magnetic properties.

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