Himalayan Journal of Science and Technology, Vol.6 (2022), 96-99

Himalayan Journal of Science and Technology

Original Article

doi: 10.3126/hijost.v6i1.50602

Electronic and magnetic properties of Half Heusler alloy NiCrSi

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Abstract

Utilizing the Quantum Espresso Package and the plane wave pseudopotential approach, the electrical and magnetic characteristics of the Half Heusler alloy NiCrSi have been investigated. Ultrasoft pseudo-potential is used for this calculation. Through our calculation, it was revealed that NiCrSi is a half-metallic ferromagnet in nature with a bandgap of 0.81eV and an effective moment of 2μB respectively. The origin of the gap is mainly due to the covalent band gap and d-d band gap in the system separating bonding states from anti-bonding states. Our calculation predicts a larger spin moment at Cr site than at Ni site which is antiparallel to the moment of Si. The hybridization of Ni- 3d and Cr-4d states can open a minority spin gap at E_f resulting in the semi-conducting nature of the minority spin band.

Article Info

Article history:

Received date: Oct 15, 2022
Accepted date: Dec 17, 2022

Keywords:
Planewave, Heusler Alloy, Half-metallic, Band structure, DOS

1. Introduction

Heusler compounds (Felser C., & Hirohaa A., 2016) are an extraordinary group of intermetallic compounds which have a peculiar property of half metallicity showing 100% spin polarization at the fermi energy. Moreover, many new properties and potential fields of applications are emerging which can revolutionize technological applications. By altering their chemical makeup, their band gaps can be easily controlled from 0 to about 4eV. They are typically represented by the generic formula X_2YZ, where X and Y are transition metals and Z is a group of elements from the III-V atomic family. In the beginning, Heusler alloys were thought to be made up of composition 2:1:1 stoichiometry. Later on, it was found that it is possible to keep one of its sublattices unoccupied giving rise to C_1b structure with the generic formula XYZ. In recent years, it has gained a lot of attention due to its possible applications in spintronics/magnetoelectronic. This is due to their half metallicity, which causes them to behave metallically in one spin channel and semiconducting in another. A very low number of states at the Fermi level is indicated by the valence band maximum, which is located only slightly above the Fermi level. This indicates 100% spin polarization at the Fermi level as required for half metal.

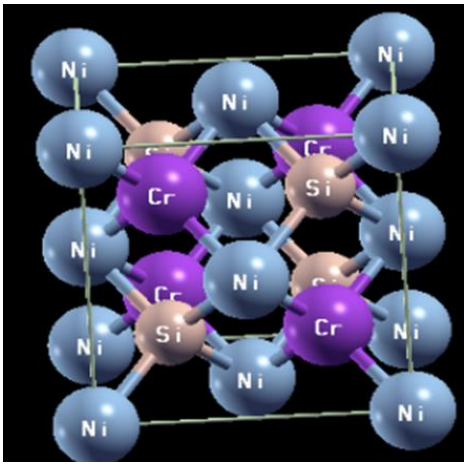

Figure 1: Conventional unit cell of NiCrSi with 16 atoms/cell

On the basis of their band structure calculation, de Groot and Bushow (Groot et al., 1983) discovered half metallicity in NiMnSb. To investigate the electrical and magnetic characteristics of the Half Heusler alloy, many sorts of research have been carried out. Nanda et al. looked at the electrical structure, chemical relationships, and magnetism of a group of half-Heusler compounds, XMZ, where X = Fe, Co, Ni, M = Ti, V, Nb, Cr, Mo, and Z = Sn, Sb. (Nanda et al., 2003). They concluded from a thoroughout investigation of numerous chemical bonding indicators that the covalent hybridization of the higher valent transition

element M is essential for the development of the d-d gap. According to a prediction made by V.A. Dinh et al., NiCrSi and NiMnSi are half metals with integer values of the total spin moment at their equilibrium lattice constants. (Dinh et al., 2010). The electrical and magnetic characteristics of NiXSb (X = Ti, V, Cr, Mn) were determined by M.P. Ghimire et al. (M. Ghimire et al., 2011), revealing that NiVSb, NiCrSb, and NiMnSb are HMF whereas NiTiSb indicates the potential for HMF.

2. Materials and Method

We estimated the electrical and magnetic characteristics of the substance under study by adopting ultrasoft pseudopotential utilizing the plane wave pseudopotential-based approach in the Quantum Espresso Package. By using the Perdew-Burke-Ernzerhof generalized gradient approximation, the exchange potential is computed (PBE-GGA). During the self-consistent field (SCF) computation, the cut-off energy for plane wave expansion is set to 110 Ry with a Monkhorst-Pack grid of 8×8×8. The density of states is computed with a denser k-mesh of 12×12×12. Force and SCF cycle convergence thresholds are set at 10^{-4} Ry/au and 10^{-5} Ry, respectively. In order to establish the ideal value for the lattice parameters, we assessed the ground state total energies for a range of lattice values between -10% and +10% of the experimental lattice parameters. The Quantum Espresso tool ev.x is then used to fit the estimated results into the Murnaghan equation of state.

3. Result and Discussion

3.1. Band structure and DOS

We use the energy minimization approach to determine the equilibrium lattice parameter value. Figure 2 depicts how the lattice parameters for NiCrSi affect the total energy variation. According to figure 2, 5.49A° is the lattice parameter that is optimal for NiCrSi. The band structure and state density are now calculated using this lattice parameter.

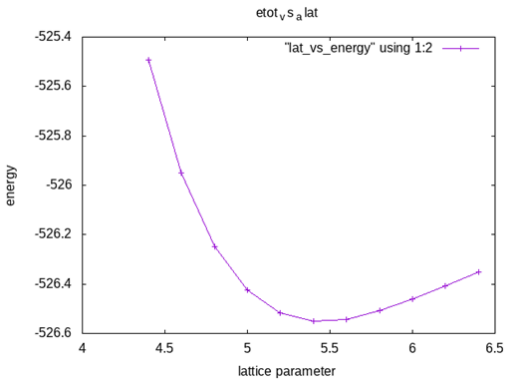

Figure 2: Plot of lattice parameter vs energy for NiCrSi

When the band structure of NiCrSi is computed, the vast bulk of the spin channel is discovered to pass the Fermi level, which indicates that up spin is metallic in nature (Kaxiras, 2003). The nature of DOS follows similar nature. In the case of minority channel band structure calculations for NiCrSi, we found a considerable band gap of 0.812 eV (Galanakis et. al., 2002). Point X has the lowest conduction band, and symmetric point Γ has the highest valence band. The presence of a tiny degree of density of states at the fermi level is indicated by the valence band maximum's location just above the fermi level. This shows that half metal requires 100% spin polarization at the Fermi level.

We can observe that the nature of DOS is virtually symmetrical for both spins from the whole and partial DOS given in fig. 3 and fig 4. The in-depth analysis of this alloy reveals that practically all of the Ni-4d is concentrated and occupied at lower energies in VB, but the Cr 3d is dispersed and firmly localized in both these regions. The minority spin states of Cr-3d are where the conduction band first appeared. In VB/CB, the third majority/minority spin states of Cr are predominant. Low DOS intensity is present in the Si-p states. A few minority Cr-3d spins are found in VB. The localized spin magnetic moment at the Cr site results from the extensive interchange spitting of Cr-3d states.

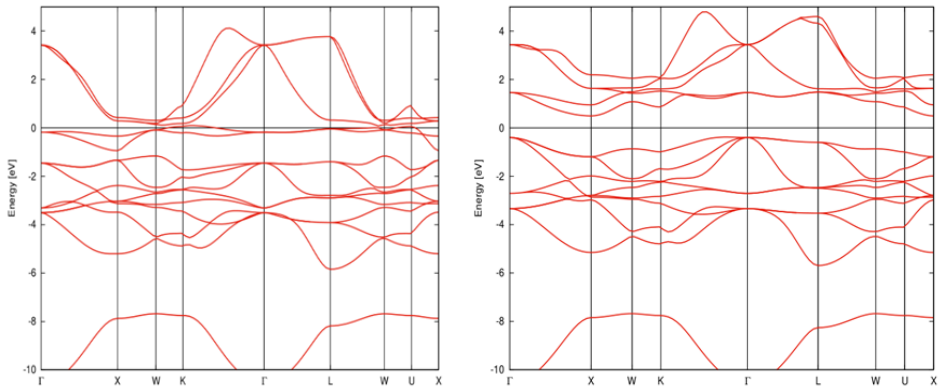

Figure 3: NiCrSi spin-up (left) and spin-down (right) channel band structures

According to our calculations, the low valent transition metal atom Cr at the Cr site as opposed to the Ni site is principally responsible for carrying out the spin moment. Each alloy's Cr-3d states have hybridized with Ni, giving each metal a small spin moment of between 0.05 and 0.15. The spin magnetic moment of the sp atoms is extremely small and anti-parallel to the moments of Ni and Cr (Dinh et. al., 2010). The s electrons of the sp element (Si) give rise to a low-lying band in both spin channels of NiCrSi that ranges in energy from 11.0 to 7.7 eV and is not depicted in the figure since it remains isolated from the other bands.

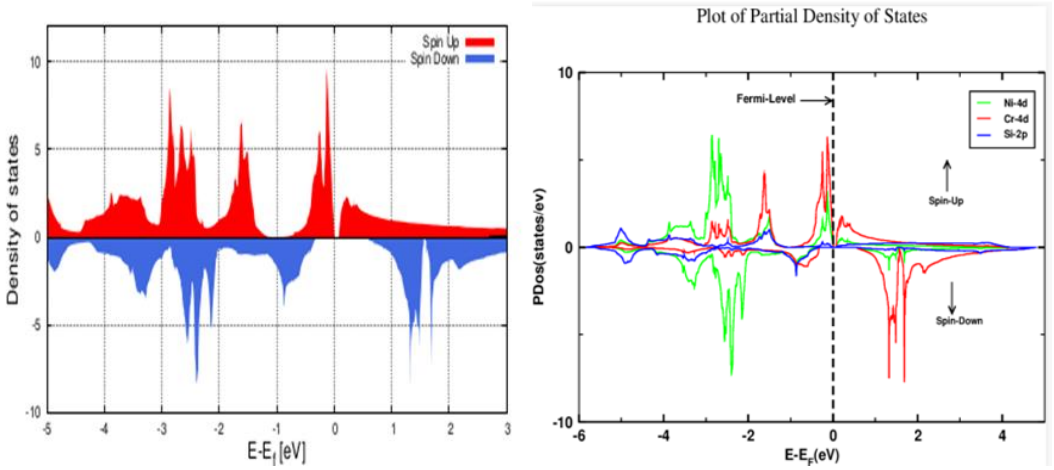

Figure 4: Total and Partial density of states of NiCrSi

A minority spin gap at E_f can be created through the hybridization of the Cr-3d and 4d (5d) states, giving the minority spin band semiconducting properties. The sp-p states are responsible for the subsequent triple degenerated band (t_{2g}) at point in the minority spin channel. After that, there are bands constructed of a Ni and Cr bonding admixture that are double-degenerated (eg) and triple-regenerated (t_2g). An indirect gap along Γ-X divides bonding hybrids from anti-bonding hybrids. Thus, there are precisely nine minority bands that are occupied. There are several bands in the majority state of this system between -6.0 and 0.0 eV where the Ni d state contributes strongly, followed by a negligible contribution from the Cr d and Si p states. Majority bands, as opposed to minority states, have 11 electrons. The final two electrons are present in states known as anti-bonding.

3.2. Magnetic property

Our calculation on the primitive cell of NiCrSi shows that the ground state magnetic structure is ferimagnetic. Ni, Cr, and Si magnetic moments at sites A and B are anti-Ferro magnetically aligned with each other. Here C site is vacant. The calculated total magnetic moment of NiCrSi is 2.00 µB, which agrees with values from the theoretical (2.0 µB) and experimental (1.95 µB) ca) calculations in the literature. The magnetic moment of individual atoms are tabulated in table 1.

Table 1: Magnetic moments of individual constituent atoms of NiCrSi for primitive cell.

Constituent atoms of NiCrSi	Magnetic moments(μ_B)
Ni(A)	0.2351
Cr(B)	1.7325
Si(C)	-0.0712

4. Conclusions

We used the plane-wave pseudopotential approach in the current calculation to examine the band structure, density of states, and magnetic moment of the Heusler alloy NiCrSi within the Density Functional Theory (DFT). From the observed result, it is found that NiCrSi is half metallic in nature. The observed results are discovered to be consistent with the earlier experimental findings. Our calculations showed that the majority spin channel is metallic in nature with overlapping bands whereas the minority spin channel is semi-conducting in nature with a band gap of 0.81eV along the symmetric directions Γ-X. The effective magnetic moment is calculated to be 2.00 μB . Our calculations revealed that the covalent band gap and the d-d band gap are mostly responsible for the gap's origin.

Acknowledgments

We are grateful to Ramesh Dhakal of Wake Forest University, Roshan Shrestha of CNRS, France, Bishnu Karki of University of Houston and Sarita Lawaju of Tribhuvan University for providing us value pieces of advice throughout our work.

Competing interests

There is no conflict of interest, according to the authors.

Funding

No funding source is available.

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