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Half metallic ferromagnetism in Ni based half Heusler alloys

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ABSTRACT

The search for emerging materials with ferromagnetic and spin flip properties has attracted widespread interest in material science. Ni based half Heusler alloys have been one of the benchmark half metallic ferromagnetic material owing to their magnetic interaction and promising figure of merit in magnetic memory element. A systematic pathway to design novel Heusler materials is by analyzing structural phase stability, electronic structure, mechanical and magnetic properties. Specifically, we carried out first principles calculations to identify the ferromagnetic and half-metallic properties of Ni based half Heusler alloys XYZ (X = Ni; Y = Cr; Z = Si, Ge, Ga, Al, In, As). The predicted phase stability shows that α-phase is found to be the lowest energy phase compared with β and γ phases. A pressure-induced structural phase transitions from α-phase to γ-phase in NiCrSi, NiCrGe, NiCrGa, NiCrAl, NiCrIn and α-phase to β-phase in NiCrAs are found. Due to the presence of d^8 and d^5 electronic configuration within Ni^{2+} and Cr^{2+} ions respectively, all the Heusler materials show half metallic behavior. Furthermore, the magnetic moments for these half Heusler alloys in all the three different phases (α, β and γ) have been reported. Our work paves the way for designing novel Heusler materials at normal and high pressure.

1. Introduction

The development of spin devices with Heusler alloys is important to both fundamental scientific research and industrial applications. Ferromagnetic materials based Heusler compounds underpin modern technologies, ranging from data storage to energy conversion and to contactless sensing. Apart from promising applications, there are several fundamental issues in half metallic and ferromagnetic half Heusler alloys, which are of general interest in the fields of solid state physics and material science [1]. It is important to analyse Ni based half Heusler alloys to find the structural phase stability, electronic structure, mechanical and magnetic properties of distinct origin upon pressure variation. In general, outstanding Heusler compounds should possess a number of desirable magnetic performance, such as large magnetization, spin polarized magneto resistive devices, spin-transfer torque magnetic memory element, transportation and processing [2]. This shows the singularity in physical-chemical trends and its search can defy intuition. The ferromagnetic half Heusler alloys of the type XYZ (X and Y = transition element; Z = sp-element) which crystallize in the $C1_b$ structure with F-43m symmetry have been studied for several years since they possess many unusual properties [3–10]. Therefore, the design of novel materials combining both magnetic and half metallic properties turns out to be vital for the development of spin electronic devices with high spin polarized charge carriers, which has motivated a continuous search for new materials. Singh et al. [3] observed that the substitution of sp-element in NiCrSi results in the minority band gap reduction. Luo et al. [4] reported that NiCrAl, NiCrGa and NiCrIn Heusler compounds were possible half metals with an energy gap in the minority spin and a completely spin polarization at the Fermi level. Dinh et al. [5–7] analysed the half metallicity and ferromagnetism in XYSi (X = Ni, Pd and Pt; Y = Cr and Mn) and NiCrZ (Z = Si, P, Ge, As, Se, Sn, Sb, Te) half Heusler alloys. Zhang et al. [8] have addressed the covalent hybridization behaviour between Ni and Cr atoms in NiCrM (M = P, As, Sb, S, Se and Te) semi-Heusler alloys. Using the full-potential linearized augmented plane wave method, Nan and Jiu [9] found that NiCrAs Heusler compound exhibits half-metallic ferromagnetism. Galanakis et al. [10] have discussed the robustness of half-metallicity in NiCrSi and NiMnSi Heusler alloys. Recently, the structural and magnetic properties of many nickel based full and inverse Heusler alloys under pressure were analysed by various researchers [11–14]. Habbak et al. [15] investigated the half metallicity and magnetic properties of half Heusler alloys PtMnSb, PtVSb, PtCrSb and PtCoSb. Behbahani et al. [16] have performed the first principles calculations to find the magnetic properties of

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Cr based half Heusler compounds. Ren et al. [17] have fabricated unidirectional crystal of Heusler Ni–Mn–Sn alloy using a modified high-pressure optical zone-melting furnace. Ma et al. [18] have used the mechanical alloying method to synthesize Ni based alloys. Wu et al. [19] have studied the half metallic and elastic properties of NiMnM (M = Sb, As and Si) alloys theoretically. Furthermore, the important problem of structural phase transition, mechanical parameters and the magnetic moments for these half Heusler alloys in all the three different phases are not yet addressed. This field is still in its infancy, and it has stimulated to study the structural, electronic, mechanical and magnetic properties of Ni based ternary Heusler compounds NiCrSi, NiCrGe, NiCrGa, NiCrAl, NiCrIn and NiCrAs with three different atomic configurations by the first principles calculations for the development of new half metallic ferromagnetic materials, by understanding the properties and practical uses of these NiCrZ half Heusler compounds (Z = Si, Ge, Ga, Al, In, As) under normal and high pressures.

2. Computational details

For exploring the physical properties of Ni based half Heusler alloys, the first principles calculations have been performed using VASP code (Vienna ab-initio simulation package). The generalized gradient approximation formulated by Perdew–Burke–Ernzerhof [20,21] (GGA-PBE) scheme is adapted to treat the exchange correlation interaction. The projector augmented wave method is used to describe the electron-ion interaction. The plane wave function is expanded with a kinetic energy cutoff of 400 eV. The Brillouin zones are sampled by Monkhorst–Pack [22] with $6 \times 6 \times 6$ k-meshes points spacing to yield accurate results for NiCrZ unit cell. When performing the calculations, both the crystal lattices and atomic positions of these half Heusler compounds are fully relaxed. The unit cell structural relaxations are carried out until the total energies are $<10^{-5}$ eV. The tetrahedron method of Brillouin integration scheme has been used to populate the electronic states in the self-consistent calculation [23]. Due to the effect of strong correlation of 3d orbital of Ni and Cr atoms, the exchange correlation potential is treated by the GGA-PBE+U scheme based on Dudarev's approach ($U_{eff} = U - J$) to address the onsite Coulomb interactions in the localized d orbitals of Ni and Cr atoms. The U-parameter corresponding to minimum energy value is found to be U = 3.7 eV for Ni and U = 4.1 eV for Cr and exchange parameter J = 0.73 eV. The crystal structure with three different atomic configurations (α, β and γ-phases) of Ni-based half Heusler alloys XYZ (X = Ni; Y = Cr; Z = Si, Ge, Ga, Al, In, Ga, As) is displayed in Fig. 1. The explicit valence electrons for NiCrZ unit cell are $3d^8\ 4s^2$ of Ni, $3d^5\ 4s^1$ of

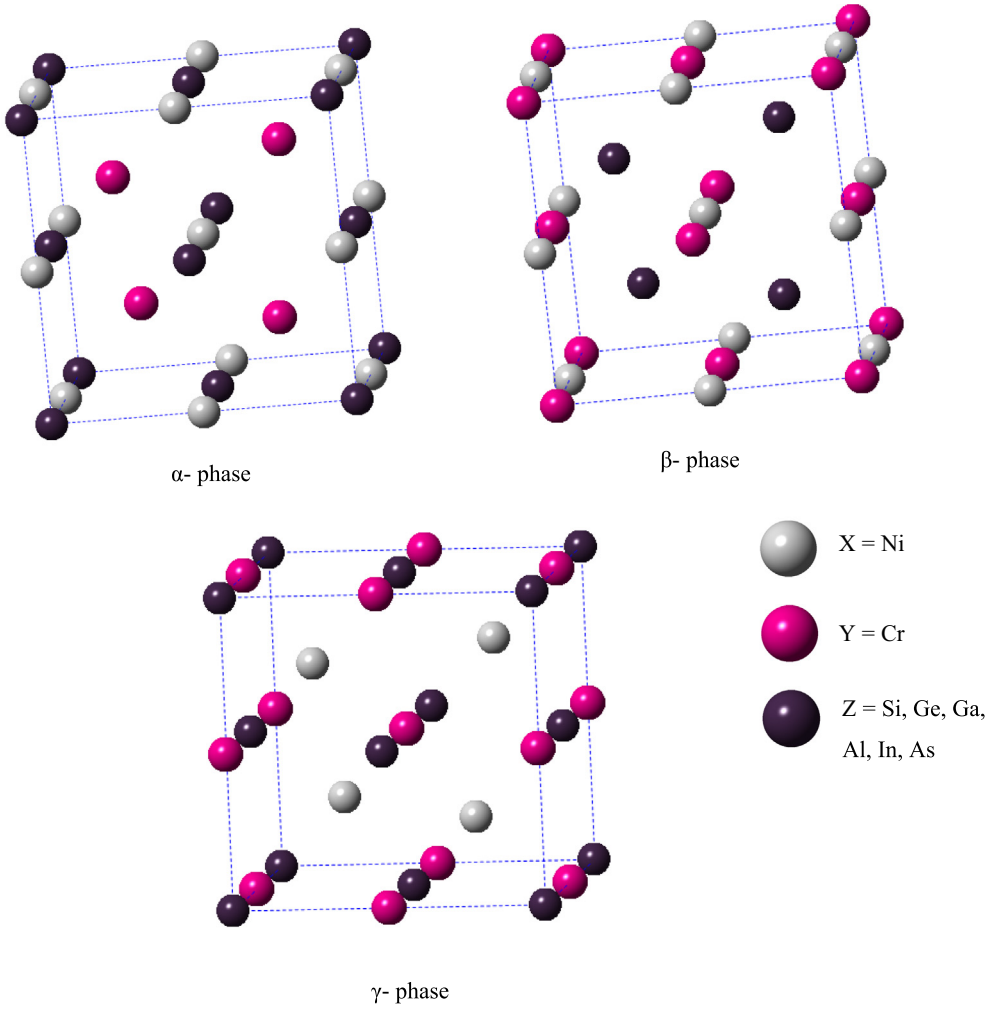

Fig. 1. Crystal structure of Ni-based half Heusler alloys in α, β and γ phases (space group F-43m) for XYZ (X = Ni; Y = Cr; Z = Si, Ge, Ga, Al, In, As).