Journal of Magnetism and Magnetic Materials 378 (2015) 1–6

Contents lists available at ScienceDirect

Journal of Magnetism and Magnetic Materials

journal homepage: www.elsevier.com/locate/jmmm

Theoretical investigation of the electronic structures and magnetic properties of the bulk and surface (001) of the quaternary Heusler alloy NiCoMnGa

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ARTICLE INFO

Article history:
Received 24 June 2014
Received in revised form
17 September 2014
Accepted 5 November 2014
Available online 8 November 2014

Keywords:
Quaternary-Heusler alloy
Half-metal
Electronic structures
First-principles

ABSTRACT

In this paper, we study the electronic structures, magnetic properties, and half-metallicity of the bulk and (001) surface of Heusler alloy NiCoMnGa. Our first-principles calculations exhibit that, within the generalized gradient approximation (GGA) of the electronic exchange–correlation functional, the quaternary Heusler alloy NiCoMnGa is a half-metallic ferromagnet at the equilibrium lattice constant of 5.795 Å with a total spin magnetic moment of 5 μ_B per formula unit. The calculated total atomic magnetic moment follows the Slater–Pauling rule. At the same equilibrium lattice constant, the half-metallicity confirmed in the bulk NiCoMnGa, is destroyed at both MnGa- and NiCo-terminated (001) surfaces and subsurfaces. Based on the magnetic property calculations, the magnetic moments of Co, Mn, and Ga atoms at the NiCo- and MnGa-terminated surfaces increase with respect to the corresponding bulk values while the atomic magnetic moment of Ni at the NiCo-terminated surface decreases.

1. Introduction

Searching for materials with high spin polarization becomes an attractive field for many researchers as an example of spintronic applications [1,2]. It is well known that a high Curie temperature and consistent electronic properties associated with Heusler alloys make these alloys of particular interest [3–5]. The 100% spin-polarization at the Fermi level (E_F) in half-metallic (HM) materials is used as a useful candidate for spin-injection devices. It displays two behaviors at the same time, one as metallic and the other a semiconducting or insulating with an energy gap at the Fermi level following the spin channel. The first time when the HM characteristic in the intermetallic half-Heusler compound NiMnSb, was predicted by de Groot et al. [6]. Many theoretical studies have been conducted to detect the transition-metal-based HM ferromagnets, such as the full-Heusler alloy Co_2CrAl [7], perovskite $La_{0.7}Sr_{0.3}MnO_3$ [8], pyrite-type CoS_2 [9], spinel Fe_3O_4 [10], rutile-type CrO_2 [11], and certain transition metal pnictides and chalcogenides in zinc-blende structure [12–14].

The $L2_1$ Heusler type (space group $Fm3m$) includes four interpenetrating face center cubic (fcc) lattices. If different atoms occupy each of the sublattices we obtain a quaternary Heusler structure with an alternative symmetry, which is the well known LiMgPdSn or Y-type structure (space group $F43m$) [15,16]. Heusler alloys can exhibit tunable electronic and magnetic properties based on their valence-electron count, so this class of materials offer a huge variety of eventualities for the design of rational materials. An important example is the quaternary alloy CoFeMnSi, which has an expected HM band structure [17]. More theoretical works on quaternary Heusler compounds CoFeCrZ done by Gao et al. [18] exposed that among all alloys investigated, both CoFeCrAl and CoFeCrSi are excellent HM ferromagnets with large HM gaps of 0.16 and 0.28 eV, respectively. They also showed that the half-metallicity of CoFeCrAl and CoFeCrSi appears to be severe against the lattice compression (till up to 7% and 4%, respectively), and the half-metalicity is preserved for CoFeCrSi and CoFeCrGe but destroyed for CoFeCrAl and CoFeCrGa when the Coulomb interaction is considered.

Recently, Felser's research group [17,19–21] found the HM ferromagnetism in many quaternary Heusler alloys such as CoFeMnZ (Z=Al, Si, Ga, Ge), NiFeMnGa, and NiCoMnGa based on some ternary Heusler compounds. They also observed high Curie temperatures (from 326 to 711 K) after fruitfully synthesizing these alloys [20,21]. Alijani et al. [21] fabricated NiFeMnGa, NiCoMnGa, and CuCoMnGa quaternary Heusler compounds by arc-melting the stoichiometric mixtures of high-purity elements in an argon

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http://dx.doi.org/10.1016/j.jmmm.2014.11.012
0304-8853/