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Electronic and magnetic properties of the (001) surface of the CoNbMnSi Heusler alloy: First-principles calculations

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ABSTRACT

In this paper, using first-principles calculations based on density-functional theory, the electronic structures, magnetic properties, and half-metallicity in the bulk and (001) surface of quaternary Heusler alloy CoNbMnSi are studied. For the bulk, the CoNbMnSi compound shows half-metallicity with a band gap of 0.5 eV in the down-spin direction at a equilibrium lattice constant of 5.88 Å. At a similar equilibrium lattice constant, the half-metallicity confirmed in the bulk CoNbMnSi, is ruined at both NbSi- and MnCo-terminated (001) surfaces and subsurfaces. Based on the magnetic property calculations, the magnetic moments of Mn and Nb atoms at the (001) surfaces increase with respect to the corresponding bulk values, while the magnetic moment of Co and Si atoms decreases. The spin-polarization ratio clearly decreases below 75% for (001) surfaces and subsurfaces of the CoNbMnSi alloy.

1. Introduction

The effective spin injection from a ferromagnet to a semiconductor is very essential for the improvement of the performance of spintronic devices [1], and thus materials with high Curie temperature, high spin polarization, and a compatible lattice structure with conventional semiconductors are required for application as a spintronic material. Half-metallic (HM) ferromagnets [2] demonstrate total (100%) spin polarization at Fermi level because the electronic structure is metallic in only one of the two spin channels. They are seen as the promising candidates as spin injection materials. Consequently, more and more HM ferromagnets with multiple structures have been predicted theoretically by first-principles calculations or proved experimentally in the past 35 years [3–7]. The spin-polarization is 100% at the Fermi energy (E_F) in the HM materials. It reveals two demeanors at the same time, one as a semiconductor or insulator with an energy gap at the Fermi energy and the other as metallic following the spin channel. Research on HM ferromagnets is rapidly growing since its prediction for NiMnSb in 1983 by de Groot and his collaborators [6]. Many theoretical studies are seen in different classes of materials, like the full-Heusler alloy [7], perovskite [8], pyrite-type [9], spinel [10], rutile-type [11], and certain transition metal pnictides and chalcogenides in zinc blende structure [12,13].

The $L2_1$ Heusler phase (space group 225, *Fm3m*) contains four interpenetrating face center cubic (fcc) lattices. If disparate atoms occupy each of the sublattices a quaternary Heusler structure is gained with an alternative symmetry, which is the renowned LiMgPdSn or Y-type structure (space group 216, *F43m*) [14,15]. Heusler compounds can illustrate tunable electronic and magnetic characteristics based on their valence electron count, so this group of materials offer a greater variety of possibilities for the design of rational materials. An important example is the quaternary alloy CoFeMnSi, which has an expected HM band structure [16]. More theoretical works on quaternary Heusler compounds CoFeCrZ conducted and experimented by Gao et al. [17] exposed that among all alloys detected, both CoFeCrAl and CoFeCrSi are excellent HM ferromagnets with huge HM gaps. They also revealed that the half-metallicity is ruined for CoFeCrAl and CoFeCrGa when the Coulomb interaction is regarded. At present, the limit of the half metals of a Heusler structure has been expanded to the compounds composing and including 4d elements [18–20], especially Co-based Heusler compounds. Co_2MnSi and Co_2FeSi compounds with a Hg_2CuTi type Heusler structure have been proved to be half metals based on first principles calculations, which have overtly enriched the potential implementation of Heusler alloys. Also, the quaternary Heusler alloys CoZrMnSi, CoTcMnSi, CoRhMnSi, CoFeCrSi, CoZrFeSi, and CoNbFeSi have been affirmed to be half metals. Among these quaternary Heusler alloys mentioned earlier, CoAgMnSi, CoMoMnSi,

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