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Research articles

Half-metallicity of (0 0 1), (1 1 0) and (1 1 1) surfaces of zinc-blende MnBi and their interfaces with HgTe: A first-principle investigation

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ABSTRACT

A first-principle study of structural, electronic and magnetic properties of the bulk on (1 1 1), (1 1 0), and (0 0 1) surfaces of zinc-blende manganese bismuth and the MnBi/HgTe (0 0 1) and (1 1 0) interfaces is undertaken. In case of the bulk, the compound exhibits half-metallicity with an energy gap of 1.27 eV in the minority-spin direction at the equilibrium lattice constant of 6.412 Å. The results show that the half-metallicity of this bulk is well preserved on the surfaces considered here except for the Bi-terminated (0 0 1) and Mn-terminated (1 1 1) surfaces. Moreover, we find that the spin magnetic moments at the (1 1 1), (0 0 1) and (1 1 0) surfaces increase compared to those of the bulk MnBi, while they decrease on the (1 1 1), (0 0 1) and (1 1 0) subsurfaces. As we calculate the adhesion energy, it is found to be the most stable interface. We find out as will that the Bi-Te(0 0 1) configuration is the most stable between the two possible configurations of the MnBi/HgTe (0 0 1) interface. Regrettably, interfacial configurations show that the half-metallicity of bulk MnBi is ruined for all possible configurations.

1. Introduction

Half-metallic (HM) ferromagnets which display metallicity solely in one of the two spin states and are awaited to show a 100% spin polarization around the Fermi energy, are seen as the most promising candidates of spintronics materials [1]. Spintronics have attracted considerable attention as they display unique opportunities for a new generation of multifunctional devices that employ conventional charge-based microelectronics with the addition of the spin degree of freedom [2]. The correlation of an electron charge to spinning has led to such interesting implementations as "spin field influence transistors [3]," "spin valves [4]" and "spin qubits [5]."

Groot and his collaborators first detected the HM ferromagnet in the half-Heusler compound NiMnSb [6]. Thereafter, several kinds of alloys, such as the half- and full-Heusler alloys [7–9], perovskite [10], rutile structure CrO_2 [11], the transition-metal pnictides and chalcogenides [12,13], and some diluted magnetic semiconductors have been found to be HM ferromagnets [14,15]. The spin injection from the ferromagnet to semiconductors requires well-conducting ferromagnet with a high Curie temperature and a high spin polarization (~half metallic). Interestingly, MnBi is a perfect candidate as a spin injector because of its high Curie temperature, high coercivity with rectangular hysteresis loop, large perpendicular room temperature anisotropy in thin films, potential to be half metallic in the zinc-blende (ZB) structure, and stable ferromagnetic phase in the NiAs structure [16].

In the past years, there has been a growing interest in diluted magnetic semiconductors, for they are promising materials for innovative spin-based devices. Some theoretical calculations have predicted that MnBi would exhibit a half-metallic ferromagnetism in the ZB structure [17–19]. In half-metallic systems, there is only one electronic spin direction at the Fermi level and subsequently such systems possess unique characteristics and are the ideal compounds for spin electronic devices. In theoretical studies of Mn pnictides, the influence of uniform volume changes on magnetic properties has been considered. Since the bulk ZB structure of Mn alloys is unstable, the epitaxial growth of Mn pnictide formation of nanostructures, such as nanodots embedded in semiconductor superlattices with semiconductors or thin films, is expected to be achieved. In such cases, strains inside the films, nanostructures, superlattices and multilayers are expected to play a critical role in the stability and other electronic and magnetic properties. So far, there are many studies on the bulk ZB structure of MnBi, but to the best of our knowledge, the MnBi alloy has never been investigated theoretically in the form of thin films or multilayers. These properties are very important for practical

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