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The half-metallic properties of bulk and the (111), (110) and (001) surfaces for the full Heusler alloy Zr_2VIn

Jabbar M. Khalaf Al-zyadi [a,*], Hassan I. Asker [a], Kai-Lun Yao [b,c]

[a] Department of Physics, College of Education, University of Basrah, Basrah, 6100, Iraq
[b] School of Physics and Wuhan National High Magnetic Field Center, Huazhong University of Science and Technology, Wuhan, 430074, China
[c] International Center of Materials Physics, Chinese Academy of Sciences, Shenyang, 110015, China

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ABSTRACT

Spin polarization and half metallicity are the basic properties of spin electronics devices. The electronic and magnetic characteristics of the $CuHg_2Ti$-kind structure Zr_2VIn full Heusler alloy in the bulk and (111), (001) and (110) surfaces are explored using the first-principles investigation based on the density functional theory. The results show that the bulk Zr_2VIn alloy achieves a ferromagnetic half-metallic characteristic with an energy gap of 0.3 eV, while the half-metallic characteristic is destroyed at all surfaces. It is noted that this compound shows 100% spin polarization at the Fermi level in the spin-up channel. The current communication also reveals that a total magnetic moment of the Zr_2VIn alloy is equal to $2\mu_B$. The atomic relaxation of (111), (001) and (110) surfaces of the Zr_2VIn compound are also discussed. The Zr(2) atom at (001) surface exhibits the highest spin polarization of 87.79%, a matter that opens the way for several applications related to designing a giant magnetic resistance.

1. Introduction

Changing physical properties of materials can play a significant role in the development of many technological applications including medical applications, chemical stirring, physiology, biophysics, and surfaces science [1]. In the last three decades, half-metallic (HM), ferromagnetic materials have been considered as fabulous materials and they have attracted a lot of the research interest, due to their possible applications in spin electronic devices (also known, as magnetoelectronics) [2]. Half-metallic ferromagnets are metallic at one of the two spin orientations, whereas they behave as semiconductor under the opposite spin orientation. These materials exhibit a 100% spin polarization at the Fermi level. De Groot et al. discovered the first HM ferromagnet in 1983 when they investigated the band structure of the semi-Heusler alloys NiMnSb and PtMnSb [3]. The half-metallic materials have wide applications in several fields, for example, magnetic sensors, tunnel junctions, spin valves, and the primary materials in electrodes [4,5]. Full Heusler composites are classified as possible candidates for spin electronic devices, because of their high magnetic moments and Curie temperatures, in addition to identical structures of the classical semiconductors [6]. These alloys have the general formula of X_2YZ, which has X and Y sites occupied by transition metals and Z by a main group element. Other researches focused on Heusler compounds that included 3d transition metal elements such as Co_2, Fe_2, Cr_2, V_2, Ti_2, and Sc_2 based alloys [7–19]. Recently, new HM Heusler alloys were developed to involve 4d transition metals such as Zr_2YAl (Y: Cr, Mn, Fe, Co, Ni) [20], Zr_2MnZ (Z: Al, Ga and In) [21], Zr_2NiZ (Z: Al, Ga) [22], Zr_2YZ (Y: Co, Cr, V, and Z: Al, Ga, In, Pb, Sn, Ti) [23], and Zr_2IrZ (Z: Al, Ga, In) [24], where X is the 4d transition metal element while Y is the 3d transition metal element. Most of the half-metallic ferromagnetics are used to shape thin films or multilayers in magneto electronic devices. However, the surfaces in thin films or multiple layers usually destroyed the half-metallic property [25–28]. Al-Zaydi et al. detected a half-metallic ferromagnetism behavior in bulk Mn_2CoSn with a $CuHg_2Ti$ structure, which was destroyed at both the Mn(2)Sn- and Mn(1)Co-terminated (001) surfaces [29]. Therefore, studying thin films or multilayers is very important as it is not yet covered well enough in the literature. To the best of our knowledge, there are no reported theoretical or/and experimental investigations of the surfaces of the Zr_2Vin alloy.

The purpose of the present paper is to provide a theoretical study of the half-metallic, electronic structure and the magnetism of the bulk and surfaces of the Zr_2VIn compound. The study also intends to verify the possibility of achieving a high spin-polarized current in the Heusler alloys. In this paper, the HM ferromagnet of the full Heusler alloy Zr_2VIn

* Corresponding author.
E-mail address: Jabbar_alzyadi@yahoo.com (J.M. Khalaf Al-zyadi).

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