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Bulk, surfaces, and interface investigations of electronic and magnetic properties: A case of the half-Heusler alloy MgCaB



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ABSTRACT

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Keywords: MgCaB half-Heusler alloy Half-metallic ferromagnetism Surface and interface properties DFT For Heusler alloys to be used in spintronic applications, the half-metallic property must be maintained on surfaces. MgCaB is a half-metal with a magnetic moment of $1\mu_B$. Considerable magnetic moment arises from the B atoms, and the hybridization between the p orbitals of B with the s orbitals of Mg and Ca gives rise to half-metallic characteristic. Herein, the electronic and magnetic properties of the (001) and (111) surfaces and the interface are examined. Results show that the half-metal is retained only in the bulk and on the Ca-terminated (111) surface and the spin polarization is equal to 100%. However, it is destroyed in all surface ends and the interface due to the relaxation effect obtained on the atoms at these ends and at the interface. The excellent bulk and Ca (111) surface half-metal properties of this new material indicate its potential applications in low-power electronics.

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1. Introduction

Spintronics, a new branch of electronics, is simply the use of the degree of rotation freedom and the degree of electron charge in several functions, the most important of which are lower energy consumption, higher storage density, and faster data processing than traditional electronics [1–6]. To produce spintronic devices for special functions, we need to search for particulate matter including only one type of spin conveyors (either spin \uparrow or spin \downarrow). In 1903, a new alloy was discovered and named Heusler alloy according to its discoverer. During that time, studies on the alloy crystal structure were not possible because of the unavailability of the necessary measuring tools. After this discovery in 1934, Bradley and Rodgers [7] discovered that the Heusler alloy Cu₂MnAl was an ordered structure with an L_{21} phase comprising four lattices of overlapping face centered cubic (FCC). Then, in 1969, Webster announced the structural and magnetic properties of Heusler alloys [8]. After a period of nearly two to three decades, research into the various properties of Heusler alloys was accelerated in 1983 with the discovery of half-metallic ferromagnetism (HMF) in NiMnSb alloy [9]. To date, numerous half-Heusler alloys have been found. Heusler alloys are classified into three basic groups, namely, half Heusler, full Heusler [10] (divided into normal and

inverse) [11,12], and quaternary Heusler [13]. In recent studies, several new Heusler alloys have been found in half-metallic materials with a high Curie temperature (T_C) and magnetic moment. The electronic and magnetic properties of new Heusler alloys are fundamentally important for spintronic devices. Semi-metallic materials can be used as thin films or multilayers, so the study of the surface properties of Heusler alloys is necessary for the development of electronic devices based on this type of material. In recent years, a new type of HMF material known as d⁰ or sp compounds has been studied. This type does not contain a transition metal [14,15]. Among Heusler materials, d⁰ Heusler alloys exhibit very suitable properties, such as large HM band gap (G_{HM}), relatively high T_C , and particularly low magnetic moment to prevent stray flux and power loss for spintronic devices [15,16].

Verifying the electronic and magnetic properties of surfaces is important as they often differ from those of their bulk structures. The same is true for the HM property, which may disappear on the material surface [17,18]. Therefore, for an HM to be used as a spin valve in spintronics, the surface must also have a HM property. Little research has been conducted on the surface and interface properties of some half-Heusler alloys, most of which do not preserve HM properties on surfaces [10,17]. For example, HM is destroyed in all surfaces (001) at Fe terminated and in (111) both Fe and Cr terminated of FeCrSe and the CrSe-terminated (001) and Se-terminated (111) surfaces keep the HM property [10]. In the present study, we investigate the properties of bulk, (111) and

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Fig. 1. (a) Total energy versus lattice constant for MgCaB, and (b) change in lattice constant in relation to the change in Eg at the E_F.

(001) surfaces, and AlSb interface with Ca-terminated (111) surface of MgCaB half-Heusler alloys.

2. Computational method

First-principle calculations are performed to obtain structural, electronic, half-metallic and magnetic properties by using density functional theory [19]. WIEN2K code is used to solve Kohn–Sham equations with GGA-PBE approximation [20,21]. Reciprocal space integrations are accomplished over Monkhorst–Pack k-point meshes of $15 \times 15 \times 15$ for the bulk and $15 \times 15 \times 1$ for the slab surface and interface, respectively. The radii R_{mt} of the muffin tins (MTs) are considered to be 2.5 a.u. for all atoms (Mg, Ca, B, Al, and Sb) in bulk, surfaces, and interface, respectively. We used $R_{mt} \times K_{Max} = 8.5$ and set the angular momentum expansion to be l = 10 in the MTs. The self-consistent field calculation iterations are less than 10^{-5} Ry per formula unit.

3. Results and discussion

3.1. Bulk properties

As aforementioned, Heusler's triple alloys or half-Heusler's comprise three interlocking FCC sub-lattices occupied by different types of atoms. The type of space-group lattice for this type is No. 216, with Ca, B and Mg atoms occupying the coordinates (0, 0, 0), (0.25, 0.25, 0.25), and (0.5, 0.5, 0.5), respectively. We find that the equilibrium lattice constant for this compound is 6.27 Å (Fig. 1(a)). An affinity lattice constant exists with the value found in a previous study [22]. Consequently, little change occurs in the energy gap. Additionally, the Fig. 1(b) shows the energy gap of the MgCaB alloy depending on the lattice constant, because the energy gap in the half-metallic material is important to spin electronics applications. We note that the MgCaB alloy has a half-metallic demeanor between (5.7 Å and 6.8 Å) of the lattice constant values. Also, the Fermi level is closer to the valence band, so this alloy can lose the half-metallicity characteristic when exposed to any kind of effects such as pressure or temperature. It is evident that the energy gap vanishes when the lattice constant increases to 6.8 Å, and thus the Fermi energy crosses the conduction band at the spin-up

state. Finally, an increase in the lattice constant of more than 6.8 Å causes the DOS to move towards regions of high energies, thereby destroying the half-metallic characteristic.

The structure is HMF with semiconductor property in spin \uparrow channel and energy gap equal to 0.735 eV. The metal property in a spin \downarrow channel (Figs. 2(a) and 2(b)) shows the spin-dependent band structure and the total and partial density of states (DOS) for the atoms. This compound is an HMF with SP = 100% at the Fermi level (E_F). G_{HM} is equal to the energy difference between the valence-band maximum (VBM) and the E_F of MgCaB and is equal to 0.183 eV. Evidently, with increased lattice constant, the VBM is oriented toward the direction of the E_F, opposite to the CBM that moves away from it.

One of the best methods of calculating the total magnetic moment of Heusler alloys is the Slater–Pauling base, which links the total magnetic moment to the total number of valence electrons [13,23]. According to this rule: $M = (2N \uparrow -Z_{Total}) \mu_B$, where M is the total magnetic moment, $N\uparrow$ is the number of revolutions of the up states, and Z_{Total} is the total number of valence electrons. For MgCaB, the Z_{Total} is seven electrons, as shown in the band structure in Fig. 2(b). The occupied majority states originate from B, Ca, and Mg atoms. Therefore, the total magnetic moment is 1 μ_B , as shown in Table 1, which also shows the magnetic moment of each atom separately.

With regard to thermoelectric properties, the BoltzTraP code was employed [24]. The thermoelectric properties were calculated as a function of the chemical potential μ at different temperatures (100, 300, 500 and 700 K) as indicated in Fig. 3. A value of $\mu = 0$ indicates an unopened system located in the middle of the band gap. The positive value ($\mu > 0$) indicates that the doping is of the n-type and the negative value ($\mu < 0$), represents the doping of the p-type. From the observation of the Fig. 3a, the Seebeck coefficient (S) tends to decrease with increasing temperature, this decrease in S due to the increase in thermal energy. This indicates that this material has good thermal performance. The maximum value of S is 2.49 mV/K at 100 K. For a high temperature 700 K, S is slightly decreased to 0.44 mV/K. The positive and negative S peaks are 2.49 and -2.21 mV/K at 100 K, 0.90 and -0.71 mV/K at 300 K, 0.58 and -0.41 mV/K at 500 K, 0.44 and -0.26 mV/K at 700 K, respectively. As we know that electrical conductivity is a



Fig. 2. (a) Spin-dependent total and partial density of states, and (b) band structure of MgCaB.

measure of a material's ability to conduct electric current. According to Fig. 3b show electrical conductivity (σ) as a function of μ at different temperatures the electrical conductivity displays similar behavior at all temperatures. It is also noted that the electrical conductivity relative to the temperatures change is at a minimum between 0.17 and 0.65 (eV), outside this range, its increases with increasing μ . We can notice that the p-type region has a higher electrical conductivity than the n-type region. Thermal conductivity (κ) is an essential thermoelectric property which characterizes the transport of energy in the form of heat instigated by a temperature gradient which follows through a material. Fig. 3c displays the evolution of the κ according to the μ at 300, 500, and 800 K. We observe that the κ for the considered temperatures is very minimal between 0.21 and 0.93 (eV). In the other μ ranges, we note that the κ increases with μ and temperature. The value of thermal conductivity is larger for $+\mu$ than $-\mu$. The performance of thermoelectric material is represented by the figure of merit (ZT), which is shown in Fig. 3d as a function of μ at different temperatures. The ZT values of half-Heusler's compound are found to increase at higher temperatures. There are two peaks of ZT in for n-type. The first maximum peak of ZT = 0.97, while for the μ values lower from 0.46 to 0.51 (eV), the ZT decrease, because, these ranges are characterized by high S, a high κ and low σ . According to obtained figure of merit (ZT) that stay around (0.91–0.97) in a very wide temperature range (0–700 K), see Fig. 3d, the thermoelectric applications for the MgCaB alloy are very possible at low and high temperatures.

3.2. Surface properties

Symmetric slabs with an odd number of layers are used to simulate the (111) and (001) surfaces of half-Heusler's alloys. According to the types of atoms present on the surface, three (111) surface ends of MgCaB are Mg-, Ca-, and B-terminated surfaces, as



Fig. 3. (a) The Seebeck coefficient (S), (b) electrical conductivity, (c) electronic thermal conductivity, and (d) the figure of merit (ZT) as a function of the chemical potential at different temperatures for MgCaB. (For interpretation of the colors in the figure(s), the reader is referred to the web version of this article.)



Fig. 4. (a) The crystal structure of MgCaB bulk, (b) Mg-terminated (111), (c) Ca-terminated (111), (d) B-terminated (111), (e) CaMg-terminated (001), and (f) B-terminated (001) surfaces.

shown in Fig. 4 (b), (c) and (d). It is also noted from Fig. 4 (e) and (f) that the (001) surface has two ends. Slab thickness is selected such that the atoms in the central layers behave almost identically to the atoms of the bulk; thus, they have the same properties. With increased slab thickness, the behavior of the central atoms approaches that of the bulk atoms. However, increasing the num-

ber of atomic layers means increasing the amount of calculation, which is why thicknesses must be carefully selected to simulate the surfaces. The number of layers that we have selected for the (111) surface is 19 layers and the (001) surface is 13 layers. An equal 15 Å space is added to reduce the effect of slabs adjacent to the slabs under study. Surface atoms are known to lose some of



Fig. 5. Spin-dependent DOS of Mg at the Mg-terminated (111) surface of MgCaB, and those of Ca and B on the (1, 2) subsurface.



Fig. 6. Spin-dependent DOS of Ca at the Ca-terminated (111) surface of MgCaB, and those of B and Mg on the (1, 2) subsurface.

their neighbors according to the end of each slab. As a result, relaxation of the atoms near the surface must be conducted. In this study, the first four layers are relaxed, proving that the change in bond length owing to relaxation affects important properties, the most important of which is the ECIs and the magnetic moments of surface atoms [25,26]. Therefore, until bond-length relaxation is achieved by calculating the changes in chemical bonds at different ends of the slabs between surface (S) and interface (S-1), the increase in Mg (S)-Ca (S-1) is 0.015 Å and that for Ca (S)-B (S-1) is 0.053 Å. However, B (S)-Mg (S-1) considerably decreases to -0.154 Å at the end Mg, Ca, and B of the (111) surface, respectively. At the end B of the (001) surface, B (S)-Mg (S-1) decreases to -0.223 Å and B (S)-Ca (S-1) decreases to -0.377 Å, whereas in the end MgCa of the same surface, Ca (S)-B (S-1) decreases to -0.002 Å and Ca (S)-B (S-1) decreases to -0.293 Å. Most of the changes in length of the chemical bond between atoms occur as a result of the electronegativity of the atoms. Owing to the high electronegativity of the B atom, valence electrons are transferred from the Mg and Ca atoms to the B atom, and because of the relatively low mass of Mg, Ca, and B atoms, they move toward one another through electrostatic forces.

The representation of the DOS of atoms on the surface and the first and second subsurface layers of the slabs compared with the DOS of these atoms in the bulk are shown in Figs. 5–9. The HM property is destroyed in all ends of the surfaces except for the Ca end on the (111) surface as it retains the HM property. If the electron spin is \uparrow , it is a semiconductor; if \downarrow , it is a metal.

The calculated values of the magnetic moments of the surface, subsurface 1, and atoms of subsurface 2 layers are listed in Table 1. The change that occurs between the magnetic moments of the atoms in the bulk and those on the surface, subsurface 1, and subsurface 2 is due to the variations in the Exchange correlation interactions ECIs, which result from the relaxation of the bond length and the decrease in number of neighbors. When the closest neighbor is lost to an increase in ECIs, a decrease (increase) in bond length leads to an increase (decrease) in ECIs [25–27].



Fig. 7. Spin-dependent DOS of B at the B-terminated (111) surface of MgCaB, and those of Mg and Ca on the (1, 2) subsurface.



Fig. 8. Spin-dependent DOS of Ca at the Ca-terminated (001) surface of MgCaB, and those of Mg and B on the (1, 2) subsurface.

We conclude that a decrease in ECIs reduces the magnetic moment and vice versa. The decrease in magnetic moment and the destruction of the HM characteristic at the Mg and Ca ends on the (111) surface and on the (001) surface at the ends of MgCa and B can be attributed to the high relaxation state of the atoms on this surface. The loss of the closest neighbor of the atoms is also important in ECIs.

3.3. Interface properties

We subsequently investigate the interfacial properties of the Ca end on the (111) surface with the semiconductor AlSb on the (111) surface at both Al and Sb ends. The study of the interface between an HM and a semiconductor is very important because

most spintronic devices use HM materials to inject current into the semiconductor. The lattice constant for AlSb is 6.135 Å [28]. The number of layers used is 11 layers of the semiconductor and 19 layers of the half-metal so as two equivalent interfaces (see Fig. 10). Figs. 11 and 12 show the DOS for the interface. Results indicate that the HM property is destroyed at both ends for various reasons, the most important of which is the apparent relaxation effect of the chemical bond between atoms and the small ECIs (near E_F). These phenomena lead to a reduction in magnetic moment, which is considered a fundamental feature of HMF materials (Table 2). We calculate their interface adhesion energy γ , defined as the work of each interface region to separate the interface into two free surfaces; thus, it can be considered a measure of γ for



Fig. 9. Spin-dependent DOS of B at the B-terminated (001) surface of MgCaB, and those of Ca and Mg on the (1, 2) subsurface.

Table 1

Magnetic moments (μ_B) and spin polarization (SP) of Mg, Ca, and B atoms in different positions of the bulk, (111) and (001) slab surfaces, and in the bulk of MgCaB.

| | Atom | s (↑ / ↓) | p (↑ / ↓) | d (↑ / ↓) | Total (\uparrow / \downarrow) | M ($\mu_{\rm B}$) | SP (%) |
|----------------|-----------|-----------|-----------|-------------|-----------------------------------|---------------------|--------|
| Bulk | Mg | 1.21/1.23 | 3.19/3.14 | 0.03/0.02 | 4.44/4.38 | 0.055 | 100 |
| | Ca | 1.05/1.13 | 2.98/3.03 | 0.20/0.62 | 4.24/4.79 | 0.098 | 100 |
| | В | 0.66/1.05 | 1.16/3.13 | 0.01/0.13 | 1.83/4.14 | 0.589 | 100 |
| Mg-ter (111) | Mg (S) | 1.21/1.22 | 3.07/3.06 | 0.01/0.008 | 4.29/4.28 | 0.008 | 15.14 |
| | Ca (Sub1) | 1.05/1.05 | 2.96/2.96 | 0.18/0.17 | 4.20/4.19 | 0.012 | 38.00 |
| | B (Sub2) | 0.59/0.59 | 0.89/0.75 | 0.008/0.008 | 1.50/1.35 | 0.146 | 23.35 |
| Ca-ter (111) | Ca (S) | 1.05/1.05 | 2.96/2.95 | 0.61/0.10 | 4.17/4.10 | 0.072 | 100 |
| | B (Sub1) | 0.66/0.64 | 1.12/0.58 | 0.008/0.008 | 1.78/1.24 | 0.548 | 100 |
| | Mg (Sub2) | 1.21/1.22 | 3.18/3.15 | 0.03/0.02 | 4.43/4.39 | 0.037 | 100 |
| B-ter (111) | B (S) | 0.67/0.65 | 0.84/0.44 | 0.006/0.005 | 1.51/1.10 | 0.412 | 23.98 |
| | Mg (Sub1) | 1.18/1.18 | 3.12/3.08 | 0.02/0.01 | 4.33/4.27 | 0.052 | 2.86 |
| | Ca (Sub2) | 1.04/1.04 | 2.94/2.93 | 0.17/0.10 | 4.15/4.07 | 0.087 | 19.50 |
| CaMg-ter (001) | Ca (S) | 0.99/0.99 | 2.77/2.77 | 0.17/0.17 | 3.94/3.94 | 0.0006 | 3.21 |
| | Mg (S) | 1.16/1.16 | 3.09/3.09 | 0.02/0.02 | 4.27/4.27 | 0.0004 | 6.95 |
| | B (Sub1) | 0.66/0.57 | 0.73/0.73 | 0.009/0.009 | 1.33/1.30 | 0.0008 | 1.37 |
| B-ter (001) | B (S) | 0.60/0.58 | 0.90/0.34 | 0.006/0.005 | 1.50/0.93 | 0.0575 | 28.03 |
| | Ca (Sub1) | 1.04/1.03 | 2.93/2.90 | 0.22/0.10 | 4.19/4.03 | 0.162 | 39.68 |
| | Mg (Sub1) | 1.14/1.15 | 3.12/3.09 | 0.02/0.01 | 4.28/4.25 | 0.032 | 78.50 |



Fig. 10. The slab models used to study the MgCaB/AlSb (111) interfaces. (a) Ca-Sb (111) interface, and (b) Ca-Al (111) interface.



Fig. 11. Interface atomic DOS of the Ca(111)/Al(111) interface in AlSb.



Fig. 12. Interface atomic DOS of the Ca/Sb (111) interface in the AlSb.

the Ca/Al (111) interface and Ca /Sb (111) interface. The interface adhesion energies γ can be written as follows:

Table 2

Shows the optimized bond distances (dint) between the interfacial atoms, and the calculated adhesion energies (γ) for two possible different configurations of the interfaces studied.

| Interfacial structure | d _{int} (Å) | $\gamma~(J/m^2)$ |
|-----------------------|----------------------|------------------|
| Ca-Al | 3.09 | 1.32 |
| Ca-Sb | 2.96 | 2.43 |

4. Conclusion

(111) interface.onfiguration hasistance which isie Ca-Al has thedistance. There-the others. Seethe others. SeeAb initio calculations are used to examine the bulk, (111) and(111) surfaces, and interface of MgCaB half-Heusler alloy. MgCaBalloy is examined for the electronic, magnetic, and half-metallicproperties of bulk, (111) and (001) surfaces, and interface of Mg-CaB. The half-metallic ferromagnetic property is retained in bulkand end Ca on the (111) surface; conversely; this feature is de-

$\gamma = \left(E_{MgCaB} + E_{AlSb} - E_{MgCaB/AlSb} \right) / A$

Here, A is the interfacial area; $E_{MgCaB/AlSb}$ is the total energy of the slab of Ca/Al and Ca/Sb; and E_{MgCaB} and E_{AlSb} are the total energies of isolated MgCaAl and AlSb in the slabs, respectively. Table 2 shows the optimized bonding lengths between the interfacial atoms after relaxation and the computed adhesion energies for the various configurations of the MgCaB/AlSb (111) interface. It is noticeable from Table 2 that the Ca-Sb configuration has the largest adhesion energies due to the bond distance which is the least among the two configurations, while the Ca-Al has the smallest adhesion energies due to the long bond distance. Therefore, Ca-Sb configuration is more stable among the others. See Table 3.

Table 3

Magnetic moment (in μ_B) and spin polarization (SP) at the MgCaB/AlSb (111) interface with Ca-Al and Ca-Sb configurations, subinterfaces (marked with *), and the bulk half-Heusler MgCaB alloy.

| Interface structure | Magnetic moments (in $\mu_{\rm B}$) | | | Spin polarization % | | | | |
|---------------------|--------------------------------------|--------------|---------|---------------------|-------|--------|--------|--------|
| | Ca | Mg | Al | Sb | Ca | Mg | Al | Sb |
| Ca-Al | 0.116 | 0.002* | 0.048 | 0.015* | 38.98 | 54.29* | 78.77 | 69.62* |
| Ca-Sb | -0.009 | -0.003^{*} | 0.0008* | -0.005 | 30.59 | 82.49* | 11.60* | 11.73 |
| Bulk | 0.098 | 0.055 | 0.00 | 0.00 | 100 | 100 | 0.00 | 0.00 |

stroyed on the (111) and (001) surfaces and the interface. The destruction is largely due to the relaxation effect and the loss of nearest-neighbor atoms. With regard to the interface, the end Ca-Sb is more stable than the end Ca-Al. All of the above-mentioned characteristics mark this alloy as a appropriate promising candidate for spintronics implementations.

CRediT authorship contribution statement

Category 1

Conception and design of study: J.M.K., W.A.A., H.I.A. Acquisition of data: J.M.K., H.I.A. Analysis and/or interpretation of data: J.M.K., W.A.A., H.I.A.

Category 2

Drafting the manuscript: J.M.K., W.A.A., H.I.A. Revising the manuscript critically for important intellectual content: J.M.K., W.A.A., H.I.A.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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