Evaluation of electronic and optical behavior of the interface of Co$_2$FeAl/AlN heusler alloy

F Lahoupour$^1$,∗ and A Boochani$^2$

$^1$ Department of Physics, Sanandaj Branch, Islamic Azad University, Sanandaj, Iran
$^2$ Department of Physics, Kermanshah Branch, Islamic Azad University, Kermanshah, Iran
∗ Author to whom any correspondence should be addressed.
E-mail: f.Lahourpour@iausdj.ac.ir

Keywords: density function theory (DFT), generalized gradient approximation (GGA), heusler’s compounds, spintronic, supercell, interface

Abstract
Based on the density functional theory, the electronic, optical, and structural properties of the Co$_2$FeAl/AlN Interface have been studied. It is shown that the Co$_2$FeAl compound is a half-metal with 100% spin polarization at the Fermi level, and the growth of this compound on the AlN semiconductor changes its stability. The best interface connection from the point of view of stability occurs in the Co-Co-Al case, which has a semi-metallic and spin polarization of the interface, which candidate it for spintronic applications. The optical properties of this interface show that it can benefit medical and sensor devices because of its anisotropic optical properties at low energies. In the infrared, visible, and ultraviolet ranges, the optical energy loss functions are zero or very little, which referred to its candidate for optical applications in these energy ranges.

Introduction
In the last years, scientists dreamed of building integrated circuits to achieve great wonders such as home computers, portable communication equipment, and automatic car control [1]. But in recent years, the development of the electronics industry seems to have slowed down due to the depletion of silicon’s ability to shrink electronic devices, so research began to find new technologies and structures to replace silicon. Scientists are looking to make electronic devices and circuits as small as possible. They are ultimately trying to make a tool that works with just one molecule or a few atoms [2, 3]. The development of technologies based on the concepts of solid-state physics and the downsizing of electronic components led to the emergence of a new realm of microelectronics [4–6]. The main goal in this field is to produce micro-scale electronic circuits and components that have high-reliability coefficients and are also economically viable, of which sub-branches are nanoelectronics.

Recent studies in electronics have focused on magnetic electronics, also known as spin electronics or spintronics. In spintronics, manipulation of spin degrees of freedom can lead to increased data processing speeds, reduced power consumption, and smaller integrated circuits [7–10]. Another advantage of using the degree of spin freedom is that a fuzzy coherence can be achieved beyond the scale of electronic instruments and thus a remarkable ability to construct quantum bits [11]. The Components made based on spintronics simultaneously have the properties of magnetic materials and semiconductors. The first generation of spintronic components simultaneously began with the discovery of the effect of Giant magnetoresistance (GMR) [12, 13] in a multi-layer spin synthesis in the 1980s, which has so far been used in hard disk heads [14]. The next generation of spintronic components came from a combination of magnetic and semiconductor materials. These components with better performance speed and less energy consumption can lead to the rise of the computer industry. However, due to manufacturing and production restrictions, it has not yet reached the desired commercial operation.
Among these is an emerging family of ferromagnets called the Heusler compounds, binary compounds of the intermediate groups of four, five, and concentrated semiconductors that behave half-metallically \[15, 16\]. Half-metallic behavior means that the density of its electron states exhibits metallic behavior for one spin channel and semiconductor behavior for another spin channel, so it has a high spin polarization at the Fermi level \[17\]. This behavior has made them suitable candidates for use in spintronics and the development of new components. Studies have shown that these compounds also have a high Curie temperature due to their strong interactions between atoms \[18\]. In 1934, Bradley and Rogers showed that structures with type L21 have ferromagnetic properties at room temperature \[19\]. Their composition was a cubic lattice of copper atoms, a body-centered cubic lattice of aluminum and iron atoms that were entangled \[20\].

Heusler compounds are divided into two categories full-Heusler and half-Heusler \[21–23\]. The first Heusler alloys studied as X2YZ with L21 space group, that X and Y were selected from transition metals and Z atoms from the main group elements. Also, the Heusler XYZ alloys with the C4b space group were discovered, recently, which are similar to L21, except that one sub-lattice is empty. These compounds are commonly known as half-Heusler or quasi-Heusler alloys. Figure 1 shows the structure of Heusler compounds.

The position of X, Y, and Z atoms of full Hussler compound alloys with the L21 crystal structure is as follows:

\[
\begin{align*}
X: & (0, 0, 0) \left\{ \frac{1}{2}, \frac{1}{2}, \frac{1}{2} \right\} \\
Y: & \left\{ \frac{1}{4}, \frac{1}{4}, \frac{1}{4} \right\} \\
Z: & \left\{ \frac{3}{4}, \frac{3}{4}, \frac{3}{4} \right\}
\end{align*}
\]

However, in half-Heusler alloys with the C4b crystal structure, the X atom is not present in position \(\left(\frac{1}{2}, \frac{1}{2}, \frac{1}{2}\right)\). In most half-Heusler alloys, we see the ferromagnetic properties, which show this property even in a weak magnetic field. An example of these is the compounds with manganese atoms, which are usually in the form of X2MnZ and with a magnetic moment of 4 \(\mu_B\) \[24–27]\). Also, due to the high Curie temperature (Tc) in many Heusler compounds of the Fe2YZ family, it is possible to use them at room temperature. Today considering a new family of these compounds as Co2YZ can be used in random memory with transient spin torque (STT-MRAM). Among the known half-metals, Co and Fe-based Heusler alloys in X and Y positions, have attracted many people by strong ferromagnetic properties and Curie temperature above 600 K and a large energy gap in the Fermi level in the down spin states \[12, 28–32\]. Although extensive advances have been in the process of identifying, designing, and producing structures based on spintronic knowledge in recent decades, we still face many challenges. Thus, increasing the volume of information can lead to the discovery of new compounds or the construction of compounds that are now in the theoretical stages. Increasing information knowledge can be studied in structures such as magnetic quantum wires and magnetic quantum dots. Recently, the growth of semiconductor thin films has been a lot of attention in the spintronic industry. Because of the different behavior of atoms located at the interface than the bulk state, the study of the half-metal properties in their interface has importance in particular. On the other hand, the surface-to-volume ratio of the material increases, and the properties of the material change \[33\]. In addition, the electric potential gradient at the layer’s interface changes electronic behavior. Since
the magneto-optical Kerr effect (MOKE) of some Heusler compounds is also interesting, the magneto-optical properties of Co$_2$FeAl/AlN alloy are studied.

**Computational methods**

The structural, electronic, and magnetic-optical properties at the Co$_2$FeAl/AlN interface were executed by Wien2K cod. The calculations were performed quantitatively based on the density functional theory (DFT) and the FP-LAPW + Lo method, as well as the exchange-correlation energy approximated by PBE (Padron-Burke-
Enzerhof [34]. within generalized gradient approximation (GGA). According to the unit cell symmetry and also to reduce the computational volume, we reduced the structures from fcc to tetragonal. To reduce the interlayer and sub-layer stress, we considered the AlN lattice constant equal to 6.1 Å. Epitaxial lattice parameters were performed based on the relaxation of the interface structure of Co-Co-Al, Co-Co-N, and Fe-Al-N with 1 Dyn /a.u force in the mini-position order. The distance between the layer and the sub-layer (h) was first considered $h = (ds+dt)/2$. The ds and dt are the distances between adjacent layers in the AlN sublayers and the Co$_2$FeAl film, respectively. Finally, we reached the energy convergence for the most appropriate h. The optimal RKMax, K-point, and Gmax parameters used in the calculations were selected 8.5, 600, and 13, respectively. To enhance the accuracy, the amount of K-point in optical calculations was considered 6000.

Figure 4. DOS diagram of (a) Co$_2$FeAl and (b) AlN.

Figure 5. DOS diagrams of atoms (a) Co-Co-Al, (b) Co-Co-N and (c) Fe-Al-N at the Co$_2$FeAl/AlN interface.
Results and discussion

The full-Husler alloy unit cell of bulk structure Co$_2$FeAl has L2$_1$ space group with Vikov position occupied as Co (0,0,0), Co ($\frac{1}{2}, \frac{1}{2}, 0$), Fe ($\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$), and Al ($\frac{3}{4}, \frac{3}{4}, \frac{3}{4}$). The amounts of obtained minimum energy and equilibrium lattice constant of the Co$_2$FeAl compound are in good agreement with the results of other works [35], have been listed in table 1. The structure of the constructed cell consists of two parts, the half-metal layer of figure 2(a) and the semiconductor substrate of figure 2(b). Figure 3 shows some examples of the desired half-metal that we have grown on the substrate. Due to the symmetry in the unit cells of both materials, we reduced their structure from fcc to tetragonal, which this change reduced the calculation. As can be seen, because the arrangement of the neighbors in the boundary layers is not the same, the forces applied to them are different. Therefore, their distance from the initial equilibrium state changes.

Figure 4(a) represents the Co$_2$FeAl bulk density of states (DOS) where there is the greatest gap between the state densities of the spin channels of the majority and the minority due to the strong exchange interactions. Figure 4(b) represents the AlN bulk density of states (DOS) where there is no difference in the state densities of the spin-up and spin-down channels. As shown in figure 5, the intensity of the spin-exchange interaction is reduced by the strong potential of the atoms at the interface, especially for the Co-Co-Al interface (figure 5(a)). The interface effect causes the DOS of spin-down at the valence band edge to shift into the Fermi level. As a result, it tends from the intrinsic semiconductor to the p-type semiconductor, and we also encounter a gap reduction. As can be seen from the diagram, the magnetic semi-metallic property is well evident at the interface also away from it.

Figure 5 are shown the three possible interface DOS of Co$_2$FeAl/AlN (001) supercell Co-Co-Al, Co-Co-N, and Fe-Al-N. The DOS diagram of the Co-Co-Al contact in figure 5(a) shows that no magnetic behavior is observed at low (below of $-5$ eV) and high energy (above 6 eV). The DOS of electrons is asymmetric in the Fermi range ($-3$ eV to 3 eV), which this behavior is evidence of a magnetic and half-metallic interface. The spin interaction which causes a bandgap in the spin-down makes the Co-Co-Al contact a much more suitable half-metal for spintronic applications. In the majority spin, the shape of the resulting DOS curve appears as a saw tooth (more alternate) which is similar to the behavior of Nano systems.

At the Co-Co-N Interface of figure 5(b), as in the previous case, the polarization of the electron states at the Fermi level is less than 100% and is about 40%. In this respect, the magnetic anisotropy in the electron states is much less than the Co$_2$FeAl bulk, but in the (001) direction, this thin film is a very good half-metal. However, one of the challenges of Heusler’s thin films is the lack of 100% spin polarization at the Fermi level [36]. Among these contacts in the interface, the Co-Co-Al interface has the most half-metallic behavior and magnetic polarization, so we emphasize this one. According to the band structure diagram of the Co$_2$FeAl/AlN combination in figure 6, the Fermi level has cut the band structures in spin-up mode, so, in this case, we see a metal property. But in the spin-down, the Fermi surface is slightly touched band structures also a small gap has been seen, so in this case, the interface has the semiconductor property.
Optical properties

The optical constants are responsible for the behavior of matter in the face of incident light. The dielectric constant is one of the important optical functions with two parts, real and imaginary. Figure 7(a) shows the real part of $\varepsilon(\omega)$ in the Co-Co-N interface of the Co$_2$FeAl/AlN supercell. Below the 1 eV in the x-direction, the inclination of Re $\varepsilon(\omega)$ to an infinite value indicates the metallic behavior of the bilayer interface. Also, the negative sign of the Re $\varepsilon(\omega)$ below the energy of 3 eV and high energies means that the incident light to the interface along the x-direction does not pass the infrared and UV light regions through it, except the visible light area. But in the z-direction, the response of the interface supercell to incident light at 0 to 1 eV is quite different. In a small area of infrared radiation, from 2000 nm (0.6 eV) to 6000 nm (0.2 eV), the interface response to light behaves quite transparently and appears metallic at smaller energies. There is no difference between the Re $\varepsilon(\omega)$ in the x and z directions from 0.9 eV upwards. The light passage phenomenon with a specific frequency at a particular direction can use in infrared spectroscopy and medical instruments [37, 38], as well as the instruments and sensors of various sciences [39].

Next, as shown in figure 7, except in the energy range of 3–7 eV, the imaginary dielectric function curve for the Co-Co-Al atoms of the Co$_2$FeAl/AlN interface behaves isotropically in both directions of x and y. The difference in dielectric function in the x and z directions of the curves in the energy range of 3–7 eV indicates optical asymmetry, as well as, the peaks shown in the curves show the optical transmission at the interface. Figure 8 shows the Eloss curve of the Co-Co-Al bond of the Co$_2$FeAl/AlN interface.

Figure 7. The real and imaginary part of the dielectric function in the Co-Co-Al bond at the Co$_2$FeAl/AlN interface.

Figure 8. Eloss curve of the Co-Co-Al bond of the Co$_2$FeAl/AlN interface.
Figure 9 shows the refractive index of the Co-Co-Al bond in the interface. Due to the easy excitation of metallic electrons in the infrared energy and the metallic tendency of the compound in this region, we expect a high static refractive index. As shown in the figure, by increasing the photon energy in the infrared region, the metallic behavior of the interface decreases in the form of an exponential sawtooth curve. Also, at low energy, the refractive index in the x and z-directions are anisotropic, and from 10 eV and above reaches a constant value of about one. So from the x-ray energy range, the Co-Co-Al bond in the interface behaves like a vacuum. The reflection curve in figure 9 also confirms this behavior.

The imaginary part of the refractive index is another optical parameter. According to the definition, this parameter is the amount of light lost amplitude that occurs in the penetration of matter. As shown in figure 10(a), at the Co-Co-Al bond in the Co₂FeAl₂N interface, a high degree of extinction occurs in the x, z directions at low energies. By increasing the photon energy in both directions, at an energy interval of 3 eV up to 8 eV, it heterogeneously shows a decreasing trend. The study of the obtained absorption coefficient curve in figure 10(b) for the interface of the above compound showed that with increasing energy, the absorption rate increases in both x and z directions. This increase coincides with a decrease in reflection from this interface.

Conclusion

In this study, we investigated the property of a half-metal at the Co₂FeAl₂N interface. To obtain the electronic properties, we used the density of the electronic states and the band structure of the compound. In the section on optical properties, the studied concepts were the dielectric function, the electron loss spectrum, the refractive, and the reflection coefficients. The calculations were performed in the form of density functional theory (DFT), using the first principle calculations by the Wien2K computational code. By investigating the diagrams of the density of state (DOS) and the obtained band structure, we found the Co₂FeAl₂N interface is a magnetic half-
metallic compound. The cobalt atoms in the layer and at the interface have magnetic half-metallic properties. The iron atoms in the upper layer and at the interface have half-metallic properties, but at the interface have more metal tendencies. In this study, we identified the best interface in Co-Co-Al. Studying the Co-Co-Al interface optical properties of the Co$_2$FeAl/AlN supercell showed Re $\varepsilon(\omega)$ tends to be an infinite negative value which indicates the plasmonic fluctuations at the x-direction (energies of 3.54 eV, 4.88 eV, and 5 eV) and the z-direction (energies of 2.53 eV, 3.81 eV, and 6.88 eV) by incident light ray. The refractive index spectrum data in both the x and z-directions show anisotropy, and both reach a constant value of about 1 at energies of 10 eV and above. Therefore, from the upper energy of the x-ray range, the Co-Co-Al interface behaves like a vacuum so that no refraction occurs in the incident light. With increasing light energy, we saw a descending reflection coefficient curve which also shows the increase in the absorption of incident light. The highest loss was in infrared light, and the amount of this loss in the x-direction was more than the z-direction.

Generally, we can conclude that the Co$_2$FeAl/AlN interface is a magnetic half-metal of 60% spin polarization and good stability. Therefore, we can use this interface in spintronic applications. Finally, to produce a half-metal with high spin polarization, it is proposed to change the z atom in the composition of Heusler, wherein this study is Al. After obtaining diagrams of compounds with different atoms and comparing them, the most suitable half-metal can identify to use in the spintronic industry.

Data availability statement

All data that support the findings of this study are included within the article (and any supplementary files).

ORCID iDs

F Lahoupour @ https://orcid.org/0000-0002-4563-1434
A Boochani @ https://orcid.org/0000-0002-2383-4169

References

[1] Moore G E 1965 Cramming More Components Onto Integrated Circuits. 38 6
[2] DONOVAN P F 1965 Experimental investigations of several few-nucleon systems Rev. Mod. Phys. 37 501–11
[3] Ozakawa K, Tsiuji Y and Yoshizawa K 2020 Understanding single-molecule parallel circuits on the basis of frontier orbital theory J. Phys. Chem. C 124 3322–31
[4] Hess D W and Jensen K F 1989 Microelectronics Processing. in Microelectronics Processing 221 (Washington, DC: American Chemical Society) 1–33
[5] Brodie I and Spindt C A 1992 Vacuum Microelectronics. in Advances in Electronics and Electron Physics ed P W Hawkes 83 (New York: Academic) 1–106
[6] Kelly M J 1986 Nanometre physics and microelectronics Phys. Bull. 37 67–9
[7] Siakeng L, Mikhali M G and Rai D P 2018 Electronic, elastic and x-ray spectroscopic properties of direct and inverse full Heusler compounds Co$_2$FeAl and Fe$_2$CoAl; promising materials for spintronic applications: a DFT + U approach J. Mater. Chem. C 6 10341–9
[8] Wang Y, Shang S-L, Fang H, Liu Z-K and Chen L-Q 2016 First-principles calculations of lattice dynamics and thermal properties of polar solids J. Phys. Condens. Matter. 28 1–10
[9] Ilkhani M, Veginen M, Boochani A and Yari A 2021 Electronic structure and magnetic properties of the CoFeMnZ (Z = As and Si) Heuslers by XAS, XMCD and MOKE: A DFT study Mater. Today Commun. 26 101773
[10] Guermint Y, Drief M, Benkhettou N, Lantri T and Rached D 2018 Electronic and elastic properties of Ba$_2$HgSn and Ca$_2$HgSn rattling heuser J. Phys. Conf. Ser. 1081 012009
[11] Leuenberger M N and Loss D 2001 Spintronics and quantum computing: switching mechanisms for qubits Phys. E Low-Dimens. Syst. Nanostructures 10 452–7
[12] Terras D, M, J, Serrate D, Córdoa R and Yusaof S M 2008 Correlation between the synthesis conditions and the compositional and magnetic properties of CoZ(C21–xFe)xAl heusler alloys J. Alloys Compd. 450 31–14
[13] Candan A, Uğur G, Charifi Z, Baaziz H and Ellahiaoğlu M R 2013 Electronic structure and vibrational properties in cobalt-based full-heusler compounds: a first-principle study of Co$_2$Mnx (X = Si, Ge, Al, Ga) J. Alloys Compd. 560 215–22
[14] Kanani H, Noma K and Hong I 2001 Advanced spin-valve GMR head Fujitsu Sci. Tech. J. 37 174–82
[15] Yan P-L, Zhang J-M and Xu K-W 2016 First-principles study on the magnetic and half-metallic properties in bulk and (001) surface of Ti$_2$CoSn Heusler alloy Thin Solid Films 609 19–24
[16] Boochani A, Nowrozi B, Khodadadi J, Solaymani S and Jalali-Asadabadi S 2017 Novel graphene-like CoZVsAl (111): case study on magnetoelectronic and optical properties by first-principles calculations J. Phys. Chem. C 121 3978–86
[17] Hillebrandt B and Felser C 2006 High-spin polarization of heusler alloys J. Phys. Appl. Phys. 39
[18] Fatáty N, Boochani A, Solaymani S, Sartipi E and Ahmadian F 2018 The band offset barrier and optical properties calculation of CoZVM/GeAs(001) interfaces: a DFT study Int. J. Mod. Phys. B 32 1570270
[19] Bradley A J, Rodgers J W and Bragg W L 1934 The crystal structure of the heusler alloys Proc. R. Soc. Lond. Ser. Contain. Pap. Math. Phys. Character 144 340–59
[20] Liu C-X et al 2010 Oscillatory crossover from two-dimensional to three-dimensional topological insulators Phys. Rev. B 81 041307
[21] Kurtulus Y, Dronskowski R, Samolyuk G D and Antropov V P 2005 Electronic structure and magnetic exchange coupling in ferromagnetic full heusler alloys Phys. Rev. B 71 014425
[22] Felser C, Wollmann L, Chudov S, Fecher G H and Parkin S S P 2016 Basics and prospectives of magnetic heusler compounds. Heusler Alloys: Properties, Growth, Applications ed C Felser and A Hirohata (Springer International Publishing) 37–48
[23] Galanakis I 2016 Theory of heusler and full-heusler compounds. Heusler Alloys: Properties, Growth, Applications ed C Felser and A Hirohata (Springer International Publishing) 3–36
[24] Berri S, Mauouche D, Ibrir M and Zerarga F 2014 A first-principle study of half-metallic ferrimagnetism in the CoFeTiSb quaternary Heusler compound J. Magn. Magn. Mater. 354 65–9
[25] Jain R et al 2017 First principle calculation of half metallicity in Ti2MnSb Heusler alloy Int. J. Mod. Phys. B 29 1550175
[26] Hussain M K, Gao G Y and Yao K-L 2015 Half-metallic properties of the new Ti2YPb (Y = Co, Fe) Heusler alloys Int. J. Mod. Phys. B 29 1550175
[27] Aguilera-Granja F, Aguilera-del-Toro R H and Morán-López J L 2019 A first principles systematic study of the structural, electronic, and magnetic properties of Heusler X2MnZ with X = Fe, Co, Ni, Cu, Ru, Rh, Pd, Ag, Pt, Au and Z = Al, Si, Ga, Ge, In and Sn Mater. Res. Express 6 106118
[28] Inomata K et al 2008 Highly spin-polarized materials and devices for spintronics Adv. Sci. Technol. Mater. 9 014101
[29] Felser C, Fecher G H and Balke B 2007 Spintronics: a challenge for materials science and solid-state chemistry. Angew. Chem. Int. Ed. 46 668–99
[30] de Groot R A, Mueller F M, Engen P G van and Buschow K H J 1983 New class of materials: half-metallic ferromagnets Phys. Rev. Lett. 50 2024–7
[31] Kawashita K, Rajanikanth A, Takahashi Y K, Ohkubo T and Hono K 2007 Microstructure and spin polarization of quaternary Co2Cr1−xVxAl, Co2V1−xFexAl and Co2Cr1−xFexAl Heusler alloys Acta Mater. 55 3867–74
[32] Li Q F, Yin J G and Zhu X F 2010 Theoretical study of the electronic and magnetic properties of Co2Cr1−xFexAl J. Magn. Magn. Mater. 322 2293–7
[33] Kawasaki S K 2019 Heusler interfaces—opportunities beyond spintronics ? APL Mater. 7 080907
[34] Perdew J, Burke K and Ernzerhof M 1996 Generalized Gradient Approximation Made Simple Phys. Rev. Lett. 77 3865–8
[35] Kelekari R and Clemens B M 2004 Epitaxial growth of the heusler alloy Co2Cr1−xFexAl J. Appl. Phys. 96 540–3
[36] Merzbacher E 1997 Quantum Mechanics. (New York: Wiley)
[37] Singh S P et al 2016 Recent advances in optical diagnosis of oral cancers: Review and future perspectives. Head Neck 38 E2403–11
[38] Mascitti M et al 2018 An overview on current non-invasive diagnostic devices in oral oncology Front. Physiol. 9 1510
[39] Judd K P and Handler R A 2019 Editorial: applications of infrared methods in fluid mechanics Front. Mech. Eng. 5 66