ISSN: 2637-6067 DOI: 10.6918/IJOSSER.202010_3(10).0044

The Stability and Electron-Magnetic Properties of Fe_2Ge Film

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Abstract

The electronic structure and electron-magnetic properties of Fe_2Ge have been studied using the first principles of DFT. To discuss the effect of Fe_2Ge atomic layer number, film thickness, energy band structure, electronic density of states and other factors on the stability and electromagnetic properties of Fe_2Gefilm. The results shown that the mainly contribution of density states were came from Fe and the contribution rate more than 92%. The density states were mainly derived from Fe 3d, Ge 4p 4s, and the spin density states were include the Fe 3d spin induces Ge 4p electron transfer. The unevenly distributed charges form the occupied state and the spin polarization states in the Fe_2Ge electronic structure system. The total number of gain electron and the total number of lost electrons are not equal. Therefore, the Fe_2Ge electronic system may have Fe 3d states and Ge 4p state hybridization. The electron properties of Fe_2Ge films with different layers and thicknesses were determined by the different electron orbits of different atoms, and the contribution of the same atom's electron to the valence band or conduction band in different energy regions were primary and secondary.

Keywords

Fe_2Ge; film stability; electronic structure; first principles.

1. Introduction

As the new type of environmentally friendly electromagnetic material, Fe_2Ge compound material has high magnetization, low dielectric constant, excellent electromagnetic properties and high curie temperature. At the same time, it is compatible with traditional silicon (Si) technology and can overcome the physical quantum limit of Si [1-5]. The magnetism of Fe_2Gemainly comes from the unoccupied Fe 3d orbital. Fe_2Ge has a series of electromagnetic stability and spectral characteristics such as high magnetization, low dielectric constant and high Curie temperature [6-9]. In addition, Fe 3 d state electrons were electrons are easily affected by external field to form spin polarization, leading to changes in the structure of the electronic layer, causing new electronic states, showing novel physical properties and phenomena, such as ferromagnetism, anti-Hall effect, and giant magnetoresistance effects and other phenomena [2]. In the Fe_2Ge spin crystal structure, the vacancy charge located in iron or

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germanium was moved to form a magnetic moment Fe_2Ge. Fe_2Ge exhibits obvious magnetic transport characteristics in the z-axis direction. This magnetic transport characteristics is different from that of magnetic transport on the x-y plane. The discovery of this characteristic also has potential application value magnetic storage electronic devices [10]. In addition, the coupling orbital is also essential for the active electronic coupling structure of the spin and Fe_2Ge coupling orbit can act on the spin. The properties of spin stress bond polarized magnetic transport are closely related to spin stress.

2. Calculation Method

The hexagonal Fe2Ge lattice constant is a=b=5.0027nm, c=4.0548nm. the symmetry constraint $\alpha = \beta = 90°, \gamma = 120°$, the space group is 194 P63/MMC. There are 6atoms in each unit cell, including 2Ge atoms and 4 Fe atoms [11-13].

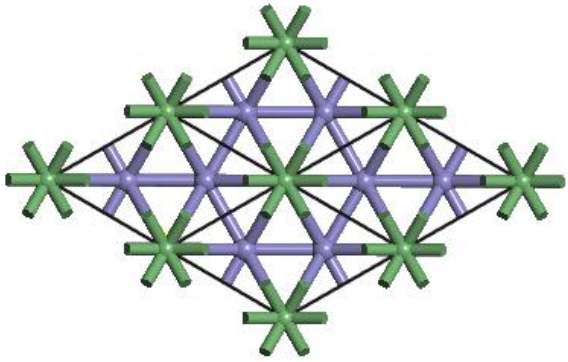

Fig 1. Fe_2Ge atoms structure schematic

The stability and electromagnetic properties of Fe_2Ge film were studied by the first principles method, all the calculations were executed using CASTEP (Cambridge serial total energy package) software package [14-19]. The interaction between lonic and electeonic interaction were calculated by Ultra Soft Pseudo Potential and Norm-conserving, respectively. The exchange-correlation potential was calculated by the PBE (Perdew Burker Emzerhof) of GGA (Generalized Gradient Approximation) method, the brillouin zone integration using Monkhorst-Pack method, the K-points was set as 4×6×3, the convergence accuracy was set 1×10^{-6}, all the calculation was in the reciprocal space.

3. Results and Discussion

3.1. The Energy Band Structure

It can be seen from the energy band structure diagram of figure 2. The figure 2 shown that the spin-up and spin-down energy band structure of Fe_2Ge compound form and asymmetric structure, the red dotted line was replaced the spin-up, the black solid line was replaced the spin-down, in this figure the red dotted line and the black solid line were not overlap, indicating that the Fe_2Ge compound is a magnetic material. The figure 2(b)~figure 2(d) were the energy band structure with different atomic layer thickness. It can be seen from the figure that as the atomic layer increases, the spin-up and spin-down the difference in the downward energy band is decreasing, indicating that the Fe_2Ge film with the thickness of a single atomic layer has the strongest magnetic properties, and its magnetic properties decrease as the thickness of the atomic layer increases.

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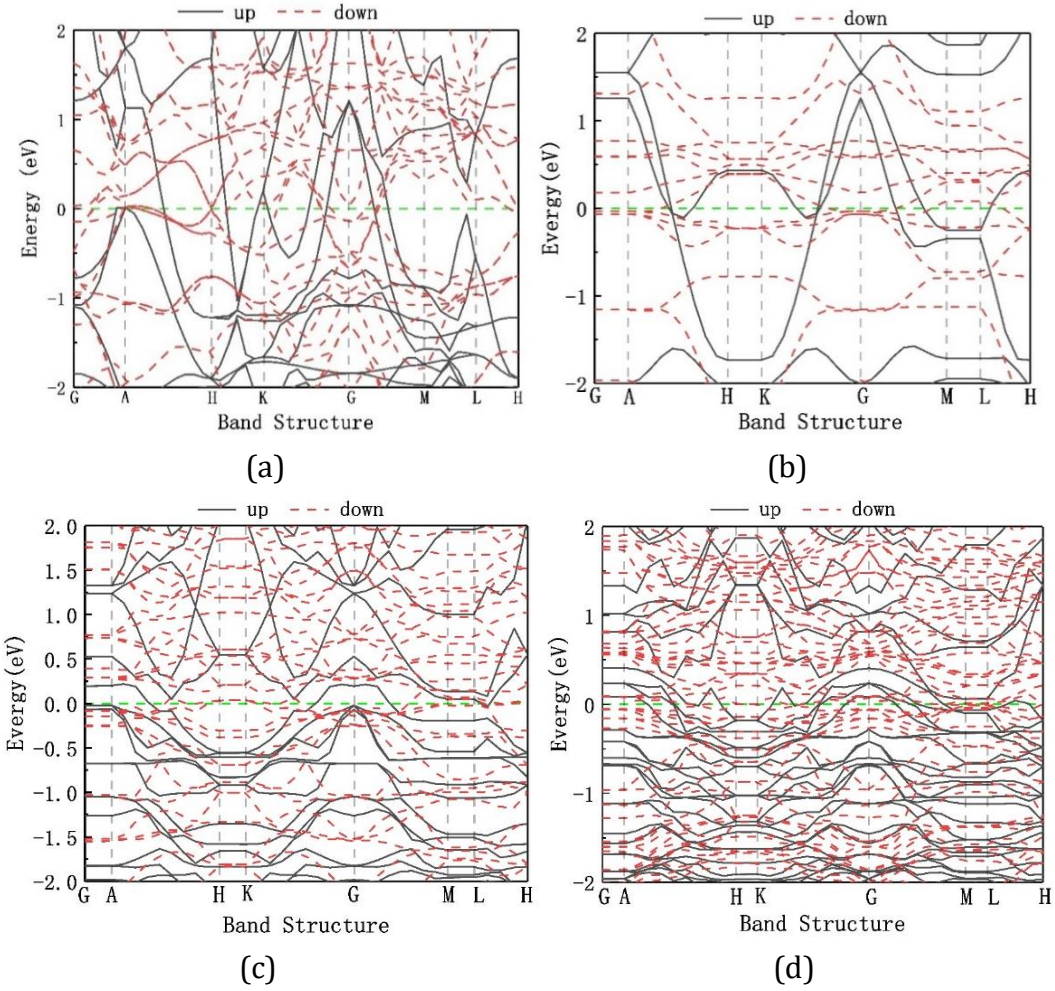

Fig 2. The band energy structure of Fe_2Ge ((a) the band structure of Fe_2Ge, (b) the band structure of Fe_2Ge thin film with an atomic layer thickness, (c) the band structure of Fe_2Ge thin film with three-layer atom thickness, (d) the band structure of Fe_2Ge thin film with five-layer atom thickness)

3.2. The Density States of Fe_2Ge

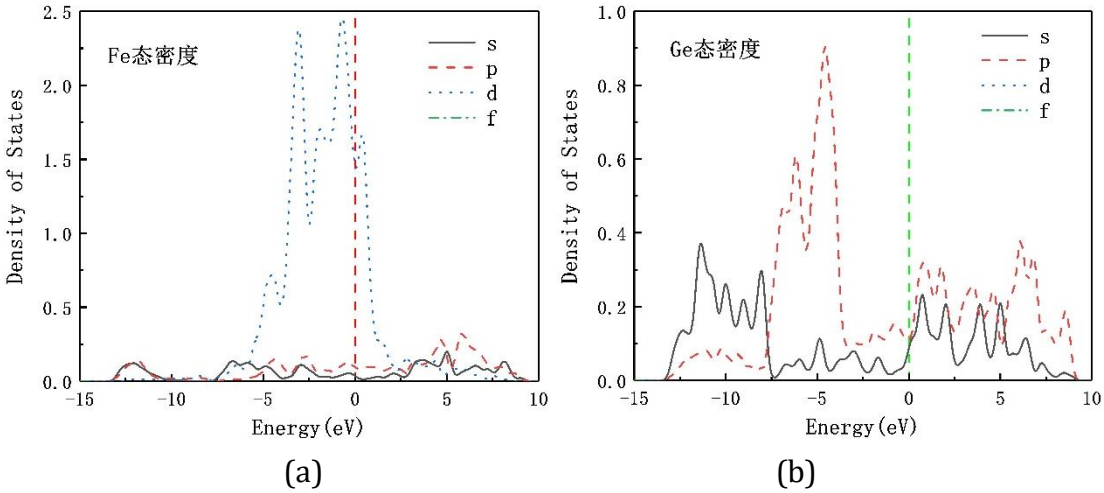

Fig 3. The density states of Fe_2Ge Fe_2Ge thin film with an atomic layer thickness ((a) the density states of Fe, (b) the density states of Ge)

Figure 3 is the partial state density of Fe and Ge of Fe_2Ge. The density states shown that in the energy range of -15eV~0eV, the main electronic states of Fe 3d and Ge 4p were contributed to

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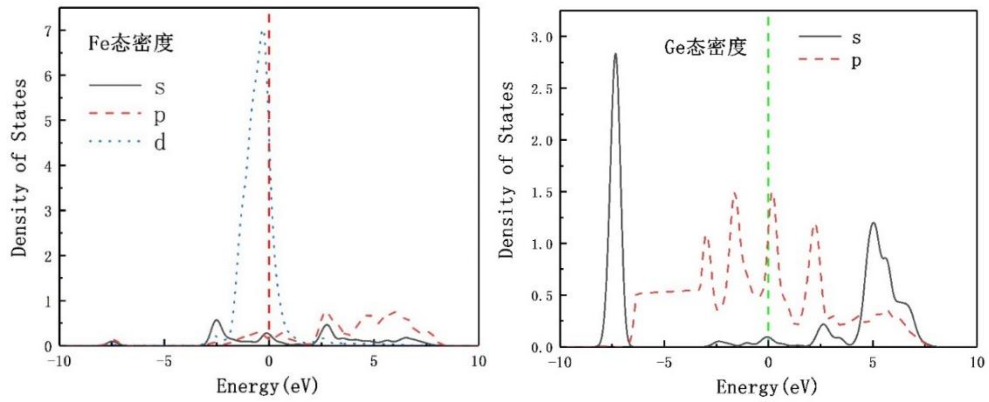
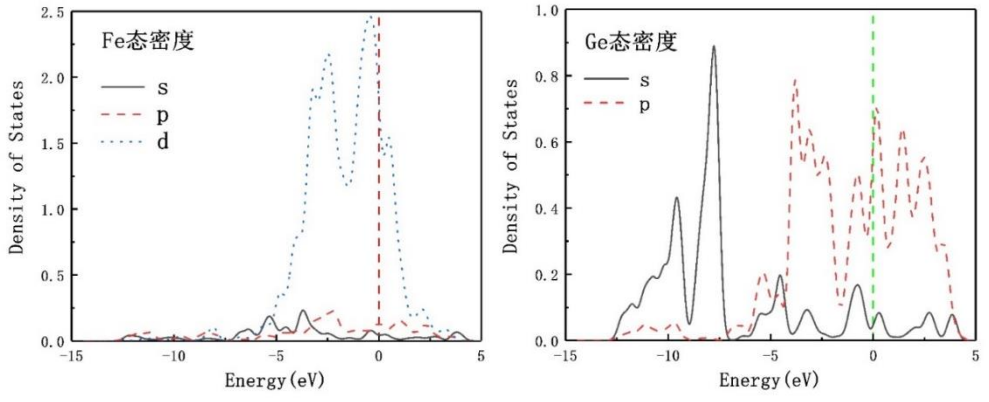
the valence band, the contributed of other electrons states to the valence band were relatively small. In the energy range of 0eV~10eV, the contribution of the electronic state of Ge 4p is greater, the contribution of the electronic state of Ge 4s was second, and the contribution of other electronic states to the valence band was relatively small. It shown that the electronic properties of Fe_2Ge were mainly determined by the electronic state of Ge 4p.



(a) (b)

Fig 4. The density states of Fe_2Ge thin film with an atomic layer thickness ((a) the density states of Fe, (b) the density states of Ge)

Figure 4(a) and Figure 4(b) were the Ge density of states and Fe density of states of Fe_2Ge with an atoms layer thickness, respectively. In the energy range of -10eV~-6.25eV, the Ge 4s state electron pair the contribution of other electronic states was relatively small. In the energy range of 0eV~10eV, the main contributions to the conduction band were the electronic state of Ge 4p and the electronic state of Ge 4s. the contribution of the individual orbitals of Fe atoms was small, indicating that electronic properties of an atoms layer of Fe_2Ge film are mainly composed of the electronic state of Ge 4s, it determined by the electronic state of Ge 4s and Ge 4p. Further analysis shown that the contribution of the electron orbits of Ge atoms to the valence band or contribution band in different energy region was divided into primary and secondary.



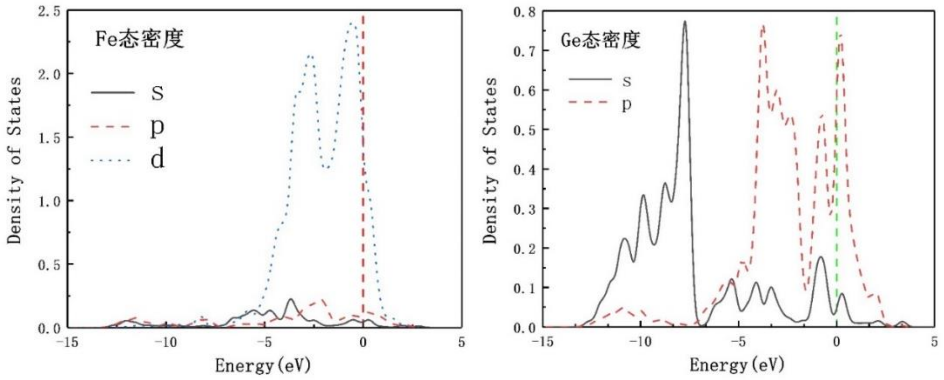
(a) (b)

Fig 5. The density states of Fe_2Ge thin film with the three-layer atomic thickness ((a) the density states of Fe, (b) the density states of Ge)

Figure 5(a) and Figure 5(b) were respectively the Ge density of states and Fe density of states of Fe_2Ge with three-layers atomic. From the figures, we can clearly see which atom was mainly composed of the valence band and the conduction band which one of the tracks contributes. In

ISSN: 2637-6067 DOI: 10.6918/IJOSSER.202010_3(10).0044

the energy range of -15eV~-5eV, the Ge 4s state contributes the most to the valence band, and the other electronic states contribute less. In the energy range of -5eV~0eV, the Ge 4p state and Fe 3d state are mainly used for the valence band. The contribution of other electronic states to the valence band is small [5]; in the energy range of 0eV~5eV, the Ge 4p state contributes more to the conduction band [5], while the other electronic states contribute relatively little, indicating the three-layer atomic layer The electronic properties of the thick Fe2Ge thin film are mainly determined by the electronic state of Ge 4p.



(a) (b)

Fig 6. The density states of Fe_2Ge thin film with the five-layer atomic thickness ((a) the density states of Fe, (b) the density states of Ge)

Figure 6(a) and Figure 6(b) were the Ge density of states and Fe density of states of Fe_2Ge with five-layers atomic, respectively. From the figure, we can see which atom was mainly composed of the valence band and conduction band. In the energy range of -15eV~-7.5eV, the Ge 4s state electrons contribute the most to the valence band, and other electronic states make little contribution. In the energy range of -7.5eV~0eV, the Ge 4p state and Fe 3d state are mainly composed Contributes to the valence band, while the contribution of the Ge 4s state is relatively small. The largest contribution to the conduction band in the energy range of 0eV~5eV was the Ge 4p state, was followed by the Fe 3d state. The resulted indicating that the electronic properties of Fe_2Ge thin films with five-layers atomic thickness are determined by the Ge 4p state and Fe 3d state.

3.3. Band Analysis

Table 1. The banding layout table of Fe_2Ge

Bond	Population	Spin	Length (A)
Fe 2 -- Fe 3	0.08	0.03	2.25793
Fe 1 -- Fe 4	0.08	0.03	2.25793
Fe 4 -- Ge 2	-0.22	0.03	2.61914
Fe 3 -- Ge 1	-0.22	0.03	2.61914
Fe 2 -- Ge 1	-0.22	0.03	2.61914
Fe 1 -- Ge 2	-0.22	0.03	2.61914
Fe 4 -- Ge 1	-0.22	0.03	2.61914
Fe 3 -- Ge 2	-0.22	0.03	2.61914
Fe 2 -- Ge 2	-0.22	0.03	2.61914
Fe 1 -- Ge 1	-0.22	0.03	2.61914
Ge 1 -- Ge 2	-58.70	14.94	2.65455
Fe 2 -- Fe 4	0.69	-0.04	2.65455
Fe 1 -- Fe 3	0.69	-0.04	2.65455

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Table 1 shows the specific bonding situation on the Fe_2Ge surface. According to the results, it is pointed out that Fe2 and Fe3 were formed a chemical bond with a bond length of 2.25793. The probability that they can bond in the entire region was 0.08, and the electronic polarization after forming the bond was 0.03; Fe2 The bond length of the chemical bond with Fe4 was 2.65455, the probability of bonding between the two were 0.69, and the electronic polarization after forming the bond was -0.04; the bond length of the chemical bond formed by Fe4 and Fe2 was 2.61914, and the bond between the two The probability were -0.22, and Fe4-Fe2 forms an anti-bonded state, the electronic polarization after bonding were 0.03; the chemical bond length formed by Ge1 and Ge2 is 2.65455, but the probability of forming a chemical bond were -58.70, and Ge1-Ge2 is also The anti-bonding state were formed, and the electron polarization after bonding were 14.94; the preliminary conclusion were that there is no direct relationship between the bonding ability of chemical bonds and the bond length, and the bonding were related to the charge transfer between atoms and the relative position.

3.4. The Charge Analysis of Fe_2Ge

Table 2. The charge analysis of Fe_2Ge

Species	Ion	s	p	d	Total	Charge (e)	Spin (hbar/2)
Fe	1	0.73	0.78	6.75	8.27	-0.27	2.61
Fe	2	0.73	0.78	6.75	8.27	-0.27	2.61
Fe	3	0.73	0.78	6.75	8.27	-0.27	2.61
Fe	4	0.73	0.78	6.75	8.27	-0.27	2.61
Ge	1	0.61	2.85	0.00	3.46	3.46	-0.05
Ge	2	0.61	2.85	0.00	3.46	3.46	-0.05

Table 2 was the charge distribution of Fe_2Ge. Through the charge distribution analysis, we can know that the electron distribution of each atom in the Fe_2Ge crystal on different orbitals. According to the results, the iron atom gets some valence electrons and carries a negative charge of 0.27. Because each Fe atom has the same gain and loss charge, the final polarization charge is also the same, both are 2.61; the germanium atom has a stronger ability to lose electrons, so it has a positive charge of 3.46, and the final polarization charge is -0.05. It is further pointed out that the relationship between the strength of gain and loss of electrons and the strength of polarization: the weaker the ability to gain electrons, the stronger the polarization; the stronger the ability to lose electrons, the weaker the polarization.

3.5. The Electron Polarization Distribution

Table 3. The electron polarization distribution of Fe_2Ge

Species	Ion	Hirshfeld Charge (e)	Spin (hbar/2)
Fe	1	-0.07	2.52
Fe	2	-0.07	2.52
Fe	3	-0.07	2.52
Fe	4	-0.07	2.52
Ge	1	0.15	0.11
Ge	2	0.15	0.11

It can be seen from table 3, the Fe atoms were negatively charged, while Ge atoms were positively charged. Iron atoms lose electrons and transfer to germanium atoms. In the new Fe_2Ge electronic structure system, the uneven distribution of electrons formed an occupied state and a spin-polarized state. Fe was an electron donor, germanium was an electron acceptor, all electrons are transferred to germanium, but increasing the total number of electrons does

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nor mean reducing the total number of electrons. Therefore, there may be hybridization of Fe 3d state and Ge 4p state in the Fe_2Ge electronic system.

4. Conclusion

In this paper, the electronic structure and electronic-magnetic characteristics of Fe_2Ge have been studied using the first principles of DFT. Discussing the effect of Fe_2Ge atomic layer number, film thickness, energy band structure, electronic density of states and other factors on the stability and electromagnetic properties of Fe_2Gefilm. The results shown that the mainly contribution of density states were come from Fe and the contribution rate more than 92%. The density states were mainly derived from Fe 3d, Ge 4p 4s, and the spin density states were included the Fe 3d spin induces Ge 4p electron transfer. The unevenly distributed charges form the occupied state and the spin polarization states in the Fe_2Ge electronic structure system. The total number of gain electron and the total number of lost electrons are not equal. Therefore, the Fe_2Ge electronic system may have Fe 3d states and Ge 4p state hybridization. The electron properties of Fe_2Ge films with different layers and thicknesses were determined by the different electron orbits of different atoms, and the contribution of the same atom's electron to the valence band or conduction band in different energy regions were primary and secondary.

Acknowledgements

This paper was supported by the science and technology foundation of Guizhou Province & Guizhou Minzu university, China (NO. LKM[2012]25), the science and technology foundation of Guizhou Province, China (NO. 1Y[2020]200, NO. 1Y[2020]205), the youth science and technology talents growth fund program of GuiZhou province education department, China (NO.KY[2018]146,) , the science and technology foundation of Guizhou Minzu university (NO.GZMU[2019]QN05), the nationalities educational reform foundation of Guizhou Minzu university, Zhejiang provincial natural science foundation of china under grant (No.LY17F010023), and Innovation Group Major Program of Guizhou Province (No.KY[2016]029).

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