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The Defects Regulating for the Electric Structure and Magnetic Properties of Fe2Ge with (0001) Surface

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Abstract

Studied the defects regulating for the electric structure and magnetic property of Fe_2Ge (0001) surface are studied by first-principle. The results show that the surface energy that is end with the Fe atomic layer was 5.3 eV·nm^(-2), the surface energy that was end with the Ge atomic layer was 7.2 eV·nm^(-2). The formed energy of Fe defect (V_{Fe}) is 2.2 eV, the formed energy of Fe anti-defect (V_{Ge-Fe}) is 8.4 eV. The magnetic of Fe_2Ge mainly comes from the spin density states of Fe 3d and Ge 2p. The magnetic moment of the Fe_2Ge (0001) perfect surface was 5.04_{uB} unit Fe_2Ge molecule, was 5.02_{uB} unit Fe_2Ge molecule of the V_{Fe} surface, and was 4.99_{uB} unit Fe_2Ge molecule of the V_{Ge-Fe} surface. The state density of spin up and spin down were decreased by defects, it was the cause of the magnetic moment reduced. In the electronic system of the Fe_2Ge (0001) surface with V_{Fe}, the periodicity of electron interaction of Ge atom was not broken, but the periodicity of electron interaction of Fe atom was broken. In the electronic system of Fe_2Ge (0001) surface with V_{Ge-Fe}, the periodicity of electron interaction of Ge atom and Fe atom were broken, so the effect of V_{Ge-Fe} was more than V_{Fe} in the Fe_2Ge (0001) surface.

Keywords

Fe_2Ge; Electronic structure; Magnetic property; Stress controlling; First-principles.

1. Introduction

Fe_2Ge compound is a new type of electromagnetic environment friendly material and has a series of electromagnetic spectrums including high intensity of magnetization, low dielectric constant and high Curie temperature (the curie temperature of Fe_2Ge is 400k, in theoretically). Above all, Fe-Ge can be extended on the silicon base[1-4], is compatible with traditional silicon (Si) process technology and able to overcome the physical quantum limit of silicon (the characteristic line of Si IC is in the range of 20 ~ 30nm) [5-7]. Based on the excellent properties of Fe2Ge, it can able to meet the requirements that including the storage information density of electron devices, the high-integrated circuit chip, and the high-speed information operation, in theoretically [8-12]. So, it has the potential application value in high speed, low power consumption, information recording and information processing devices, in the future.

Fe2Ge is a hexagonal structure that presenting the quasi-two-dimensional hexagonal structure with the Fe atom at their centers and the crystal anisotropy existed in the C axis and the perpendicular to C axis [13]. The extra-nuclear 3d of transform iron (Fe) is unfilled, and form $3d^64s^2$ extra-nuclear configuration, the extra-nuclear configuration of germanium (Ge) is $3d_{10}4s^24p^2$ [14]. The electric potential and the configuration of Fe were divided into low-spin and high-spin two parts. The center ion electron configuration was transferred between $t^6{}_{2g}e^0g$ and $t^4{}_{2g}e^0g$, the extra-nuclear electron transferred between t_{2g} and e_g orbits and was formed the new spin polarization state[15-17]. At the same time, studying the short-range structure of Fe_xGe_{1-x} found that the minimum coordination layer structure was formed between Fe and Ge

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atoms, in the nearest neighbor structure configuration [18]. The coordination layer structure is easy form a defect structure in the preparation process, and the defect structure effect the coordination structure, regularity, intensity and electromagnetic property of Fe_xGe_{1-x}[19]. But the corresponding microscopic effect mechanisms are still not systematic study.

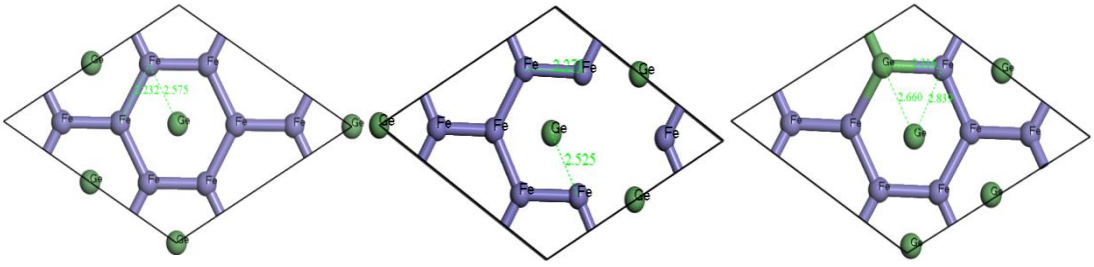
In practical, the defect structure existed in the material are unavoidable, but we can use the defect's structure designing a specific microstructure, the specific microstructure can regulate the electromagnetic properties of the materials. Studied the defects structure of material usually used the experimental method. In recent years, the first principles method has been widely used in the study of materials science, and the study results of crystal structure, polarization properties and surface properties were better with the experimental results. In this paper, we study the electromagnetic characteristics and electronic structure of Fe_2Ge (0001) surface with defects, analyze formation mechanism of the defects, reveal the influence mechanism of the electromagnetic characteristics and electronic structure of Fe2Ge (0001) surface with defects. In order to reach a consensus on the theory and the experiment provides the theoretical basis for experimental analysis.

2. Methodolgy

The CASTEP is used for structure optimization, where the electron-core interactions are described by the projector augmented wave method, the exchange correlation energy was calculated using the generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof form [20]. The cut off energy for the plane wave basis set was used to expand the Kohn-Sham, and the cutoff energy was 350eV for all calculations. The structural relaxations and total energy calculations were performed, the Hellmann-Feynman forces acting on ions were less than 10^{-2}eV/Å for all studied structures.

Iron is a transitional metals element with atomic number 26 and its outer shell ($3d^64s^2$) contains 3d electrons, the GGA approaches fails to describing the strongly correlated localized 3d electrons and predicting a metallic ground state for the iron germanide. Thereby, to account for the strong on-site coulomb repulsion among the localized 3d electron in Fe_2Ge, we used the Hubbarad-U constant describing the strong on-site coulomb repulsion [21]. The GGA+U cases were represented by the Hubbard-like term U, and the exchange term J led to an improvement of the ground state properties. Such as the band gap and the magnetic moments were improved. In the investigated, the density of states of bulk Fe_2Ge was calculated by GGA+U mothed. In this paper, the magnetism of Fe_2Ge was studied using the method of GGA+U.

The Fe_2Ge compound material is a hexagonal structure with lattice constants of a=b=0.3691nm，c=0.5401nm, the space group is P63/mmc (No.194)[22-24], the structure presenting the quasi two-dimensional hexagonal structure with the Fe atom at their centers, the molecular structure diagram was show in the figure 1.



(a) (b) (c)

Figure. 1 The molecular structure of Fe2Ge. (a)The perfect crystal structure, (b) The VFe structure, (c) The VGe-Fe structure

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3. Results and discussion

3.1. The defect formed energy of Fe2Ge (0001) surface

The Fe_2Ge (0001) surface atoms were formed the displacement structure that the Fe atomic layers and the Ge atomic layers alternating overlapped. When the number of atomic layer is odd, the end surface is Fe atom. When the number of atomic layer is even, the end surface is Ge atom.

The surface energy is given by: [25-27]

$$E_{surf}=(E_{slab}-NE_{bulk})/2A \quad (1)$$

Where Eslab is the energy of the surface model, N is the number of the unit cell in slab, Ebulk is the energy of unit cell, and A is the area of the Fe_2Ge (0001) surface.

The surface energy that is end with the Fe atom was $5.3eV \cdot nm^{-2}$, where the surface energy that is end with the Ge atom was $7.2\ eV \cdot nm^{-2}$. Compared the surface energy of two structures, we studied a more stable structure which is end with Fe atom.

The formed energy of defects was given by: [28, 29]

$$E_{form}(V_i^{\square}) = E_{tot}(V_i^{\square}) - E_{tot}(Fe_2Ge) + \mu_i \quad (2)$$

Where $E_{tot}(V_i^{\square})$ is the total energy of the super-cell containing the defect, and $E_{tot}(Fe_2Ge)$ is the total energy of the Fe2Ge perfect crystal in the same super cell. The μ_i is the chemical potential, in this paper we just consider the neutral vacancy defect.

The formed energy of Fe defect (V_{Fe}) is 2.2eV, the formed energy of Fe anti-defect ($V_{Ge\text{-}Fe}$) is 8.4eV. Compared the formed energy of two type defects, the VFe is easy formed. The molecular structure of Fe_2Ge was shown in the figure 1. The Fe atom which around the V_{Fe} was displace outside, the maximum distance is 0.05Å by V_{Fe} defect. The Fe atom which around the $V_{Ge\text{-}Fe}$ was displace inside, the maximum distance is 0.08Å by $V_{Ge\text{-}Fe}$ defect.

3.2. The effect of the magnetism and state density of Fe_2Ge with defects

ISSN: 1813-4890

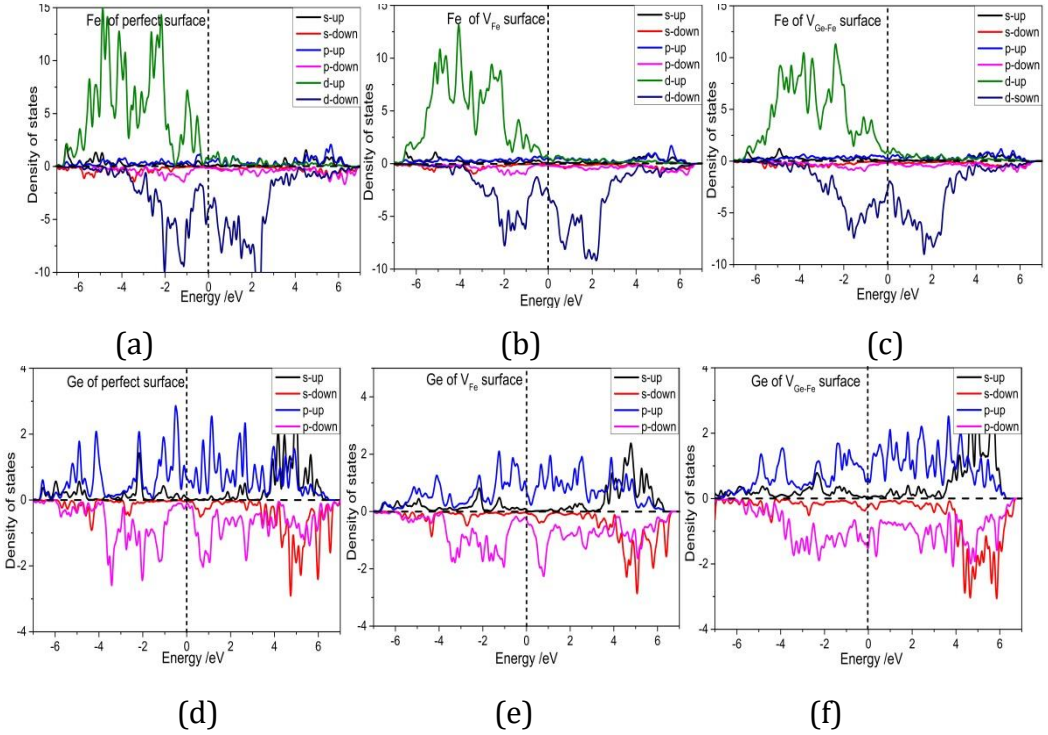

Fig.2 the density states of Fe_2Ge. (a) the density states of Fe in perfect surface, (b) the density states of Fe in V_{Fe} surface, (c) the density states of V_{Ge-Fe} in perfect surface (d) the density states of Ge in perfect surface, (e) the density states of Ge in V_{Fe} surface, (f) the density states of Ge in V_{Ge-Fe} surface

The Fe2Ge (0001) perfect surface is a hexagonal Fe ring, the magnetic moment is 5.04_{uB} unit Fe2Ge molecule, this magnetic moment was greater than the magnetic moment of Fe_2Ge perfect crystal. The result was attribute to the surface effect on the surface of Fe_2Ge (0001), the surface effect leads to the atomic ligand of the surface decreased, the surface crystal field effect increased, and the locality of Fe outer electrons was decreased. The valence electron of Fe and Ge were hybridized, the surface polarization was enhanced, and the magnetic was enhanced. The magnetic moment was 5.02_{uB} unit Fe_2Ge molecule with the VFe, the magnetic moment was 4.99_{uB} unit Fe_2Ge molecule with the V_{Ge-Fe}.

The figure 2 is the density states of Fe_2Ge (0001) surface. In the Fe_2Ge (0001) perfect surface the density states were come from the Fe 3d and Ge 2p. For the spin up state density, the spin up state density was contributed from Fe 3d in the valence band area, is less contributed to the conduction band area. For the spin down state density, the contributed of Fe 3d was mainly in the energy range of -4~4eV. The spin up density of Fe 3d and the spin down density were asymmetrical, and the asymmetrical value was formed the magnetic moment. For the Ge density states, the density states were less near the Fermi level, but it was shown a significant asymmetry, the asymmetry was due to the polarized by Fe atoms.

The state density of spin up and spin down were decreased by defects, so the magnetic property is less. In order to study the cause of magnetic decreased by defects, the influence of orbital hybridization and polarization on magnetism is considered. But Fe_2Ge is a hexagonal structure, the electron orbital hybrid effect on the electronic structure is small. So, this paper mainly analyzes Fe_2Ge interatomic bonding status in electronic structure polarization and charge transfer on the influence of the magnetic.

3.3. The effect of the atom population analysis of Fe2Ge with defects

The charge density distribution on the surface of Fe2Ge were shown in figure 3, the figure shown that the Fe_2Ge (0001) perfect surface was a hexagonal Fe ring, was formed the covalent

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bonds among the atoms, but the charge distribution was uniform. When the V_{Fe} was existed in the Fe_2Ge (0001) surface, there were three atoms that in the nearest neighbor have the unpaired electron. When the VGe-Fe was existed in the Fe_2Ge (0001) surface, the Ge atom and the nearest neighbor Fe atom were bonded by covalent bonds, but the transfers and polarization were affected by the outer charge of the atoms which the atomic radius is difference. Therefore, the symmetry of the local domain structure and the distribution of spin density around the vacancy were considered, among the charge, charge transfer and spin polarization of each atom.

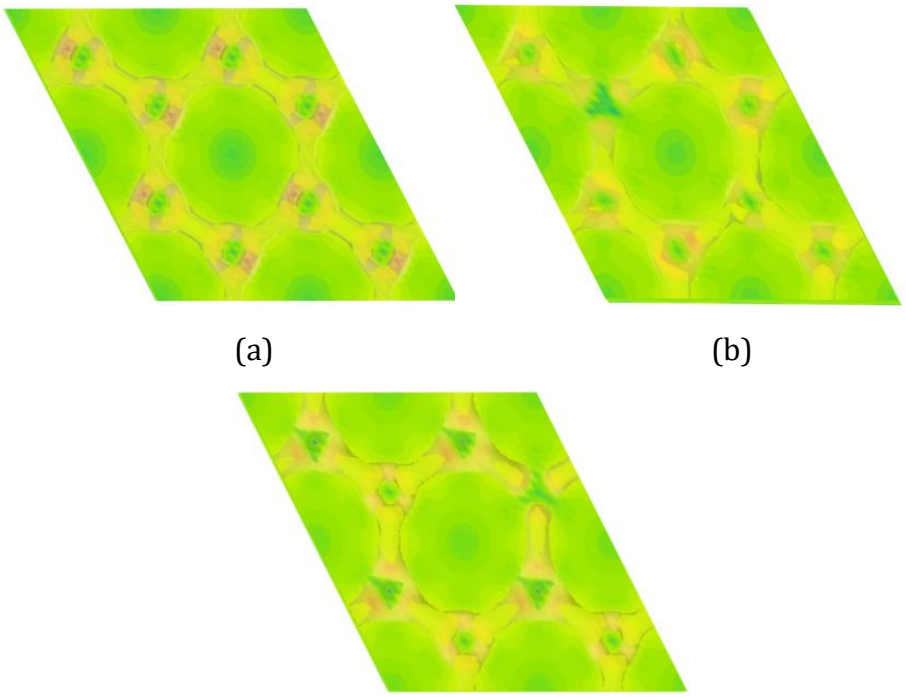

Fig.3 the charge density distribution on the surface of Fe_2Ge. (a) the charge density distribution on the perfect surface (b) the charge density distribution on the perfect V_{Fe} surface (c) the charge density distribution on the perfect V_{Ge-Fe} surface

The figure 4 is the polarization charge of Fe_2Ge (0001) surface. In the Fe_2Ge (0001) perfect surface, the polarization charges were periodically distributed on each atom of Fe and Ge. The Fe atoms were shown two polarized states. The low polarization state was 2.5e, the high polarization state was 2.65e. The Ge atoms were shown two polarized states, the high polarization state was 0.05e, and the negative polarization state was -0.22e. In the electronic system of Fe_2Ge (0001) surface with VFe, the periodicity of Ge atom was not broken, but the periodicity of Fe atom was broken. The break was main present on 8-11 Fe atoms, the high spin states of these atoms were increased, the high spin states of other atoms were almost unchanged. In the electronic system of Fe_2Ge (0001) surface with V_{Ge-Fe}, the periodicity of Ge atom and Fe atom were broken. The breaks were main present on 20-23th Fe atoms and 9th Ge atom. The figure 4 shown that the V_{Fe} was only affected the polarization of the neighbor Fe atom, but the V_{Ge-Fe} was influenced the polarization of the near Fe atoms and the entire Ge atoms, and the polarized state of Ge atom is induced by the Fe polarized. Therefore, in the way of the polarization, the influence of V_{Ge-Fe} on the electronic polarization of Fe_2Ge system was greater than that of V_{Fe}.

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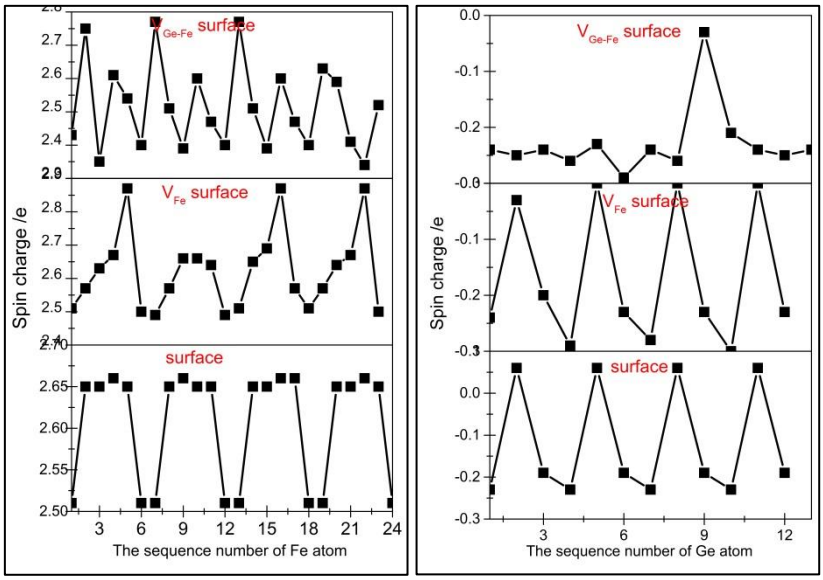
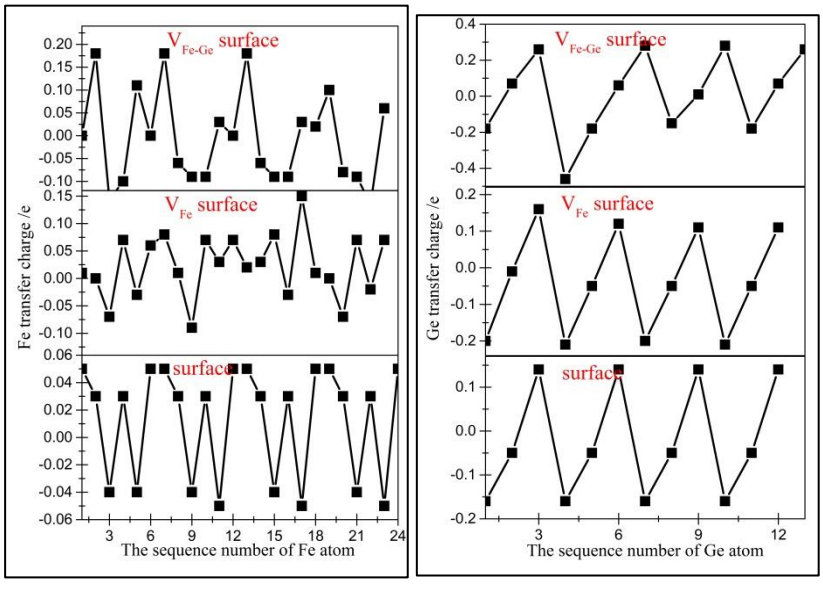


(a) (b)

Fig.4 the polarization charge of Fe_2Ge (0001) surface. (a)he polarization charge of Fe atom, (b) the polarization charge of Ge atom

The figure 5 shown that in the charge transfer system of Fe2Ge (0001) perfect surface, the charge transfer was periodically distributed on the Fe atom and Ge atom. For the Fe atoms, one of the Fe atoms was get the electronic, the other was lost electron. For Ge atom, one of the Ge atom was get the electronic, the other was lost electron. In the electronic system of Fe_2Ge (0001) surface with V_{Fe}, the transfer electronic periodicity of Ge atom was not broken, but the transfer electronic periodicity of Fe atom was broken, the transfer electronic on the Fe atom was increased. In the electronic system of Fe_2Ge (0001) surface with VGe-Fe, the transfer electronic periodicity of Ge atom and Fe atom were broken, the transfer electronic on the Ge atom and Fe atom were increased. The results show that the influence of VGe-Fe on the electronic transfer of Fe_2Ge system was greater than that of V_{Fe}.



(a) (b)

Fig.5 the transfer charge of Fe_2Ge (0001) surface. (a) the transfer charge of Fe atom (b) the transfer charge of Ge atom

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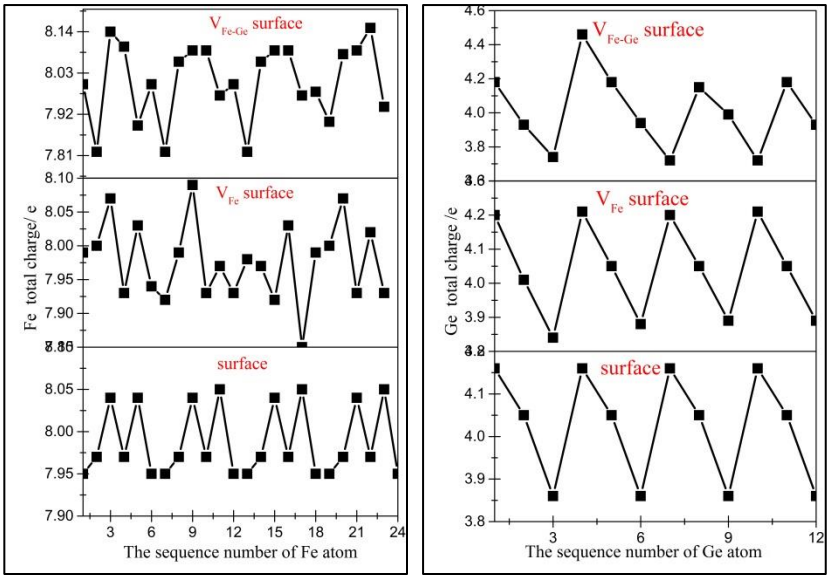
Figure 6 was the total charge of Fe_2Ge (0001) surface, analyzed the total transfer charge found that the charge transfer was not equal on the Fe_2Ge (0001) surface, there was existence the free electrons, and this part of the charge will be hybridized in the region to form a new hybrid orbital. The electronegativity which around the Fe atoms was decreased and the Ge atoms enhanced electropositive was increased by $V_{Ge\text{-}Fe}$, it leads to the covalent bonding energy of Fe-Ge decreased. The free electrons and the electronegativity were increased by the V_{Fe}.



(a) (b)

Figure 6 the total charge of Fe_2Ge (0001) surface.(a) the total charge of Fe atom, (b) the total charge of Ge atom

4. Conclusion

This paper has studied the defects regulating for the electric structure and magnetic property of Fe_2Ge with (0001) surface. The surface energy that was end with the Fe atomic layer was $5.3eV \cdot nm^{-2}$, the surface energy that was end with the Ge atomic layer was $7.2\ eV \cdot nm^{-2}$. The formed energy of Fe defect (VFe) was 2.2eV, the formed energy of Fe anti-defect (VGe-Fe) was 8.4eV. The magnetic of Fe2Ge mainly come from Fe 3d and Ge 2p, and the Ge 2p density states was polarized by Fe 3d. The magnetic moment of Fe_2Ge (0001) perfect surface was 5.04_{uB} unit Fe2Ge molecule, was 5.02uB unit Fe_2Ge molecule with the V_{Fe}, and was 4.99_{uB} unit Fe_2Ge molecule with the $V_{Ge\text{-}Fe}$. In the electronic system of Fe2Ge (0001) surface with V_{Fe}, the periodicity of Ge atom was not broken, but the periodicity of Fe atom was broken. In the electronic system of Fe_2Ge (0001) surface with $V_{Ge\text{-}Fe}$, the periodicity of Ge atom and Fe atom were broken, so the effect of $V_{Ge\text{-}Fe}$ more than V_{Fe}.

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ISSN: 1813-4890

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