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Electronic Structures and Magnetic Properties of $Fe/Si/Fe$ Trilayer

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Employing the LMTO band method, we have studied electronic and magnetic properties of $Fe/Si/Fe$ trilayer in which the z-direction is chosen to be (111) direction of $FeSi$ with B_2 phase. We have also determined electronic structure of bulk $FeSi$, as a reference material. The ground state of $FeSi$ is paramagnetic insulator with a band gap of 0.05 eV. Band structures of $Fe/Si_n/Fe$ with varying the thickness of the spacer layer reveal that the spacer layer is metallic, and the states along the growth direction do not disperse much reflecting a two-dimensional nature. Magnetic moment of Fe atom in the interfacial layer of $Fe/Si_n/Fe$ is reduced a lot as compared to the bulk value, suggesting a strong hybridization between Fe and Si states. The geometry of the Fermi surface indicates that the magnetic coupling period of ~ 8 ML (monolayers) in $Fe/Si_n/Fe$ is explained with a short Fermi wave vector of bcc Si.

1. Introduction

Since the discovery of antiferromagnetic (AF) coupling of ferromagnetic layers across metallic, nonmagnetic spacer layers, there have been extensive experimental and theoretical works [1-7] in this field. The oscillatory magnetic coupling has created widespread interest, due to potential applicability to magnetic and magneto-optical storages, and due to unusual oscillation period of the magnetic coupling. The period is on the order of 10 Å, which is much larger than the Fermi wavelength expected from simple RKKY arguments.

Many efforts have been focused on exploiting a new spacer layer material and also determining electronic and structural properties of the multilayers which exhibit AF coupling. that determine the periodicity of the coupling. In this context, using the spacer layer with a semiconductor such as Si is interesting, because the magnetic coupling through the semiconductor layer is expected to be different from the case of metallic spacer layer. Toscano *et al.* [2] observed AF coupling in $Fe/Si/Fe$ trilayers grown by evaporation at *40 K*. They found that the coupling oscillates from ferro- to antiferromagnetic with an approximate period of 16 Å. Their result clearly demonstrates that the Si layer is crystalline with either B_2 or DO_3 structure for $t_{si} < 15$ Å. Various growth experiments suggest that crystallinity of the spacer layer is crucial for the AF interlayer coupling [8, 9]. X-ray analysis by Fullerton *et al.* [8] has revealed that the Si spacer layer with thicknesses $t_{si} < 17$ Å is crystalline, while the spacer layer with $t_{si} > 17$ Å is amorphous. On the other hand, magnetic properties are thickness independent for $t_{si} > 20$ Å. They concluded that the amorphous characters of the spacer could not communicate spin information effectively.

The B_2 structure consists of two interpenetrating simple cubic substrates and becomes identical to the $CsCl$ structure for Fe_1/Si_1. The B_2 crystal structure of Si is well lattice-matched to Fe, and the lattice constant of the B_2 phase is reported by Kanel *et al.* [10] to be 2.717 Å. A common problem in preparing M/Si (M: metal) superlattices is that silicides are readily formed at the interface. Either a crystalline or a amorphous silicide compound is formed depending on the temperature and on the specific metal element in M/Si system [11]. In fact, there is no overall agreement in interface structures of Fe/Si. According to Urano *et al.* [12], the interface is abrupt with a layer-by-layer growth of an epitaxial Fe film on the Si substrate.

In this study, to investigate the characters of the semiconducting spacer layer in the $Fe/Si/Fe$ trilayer system, we have calculated electronic and magnetic structures in a series of $Fe/Si_n/Fe$ trilayer. We have also calculated the electronic structure of bulk $FeSi$ as a reference material. Electronic structures and

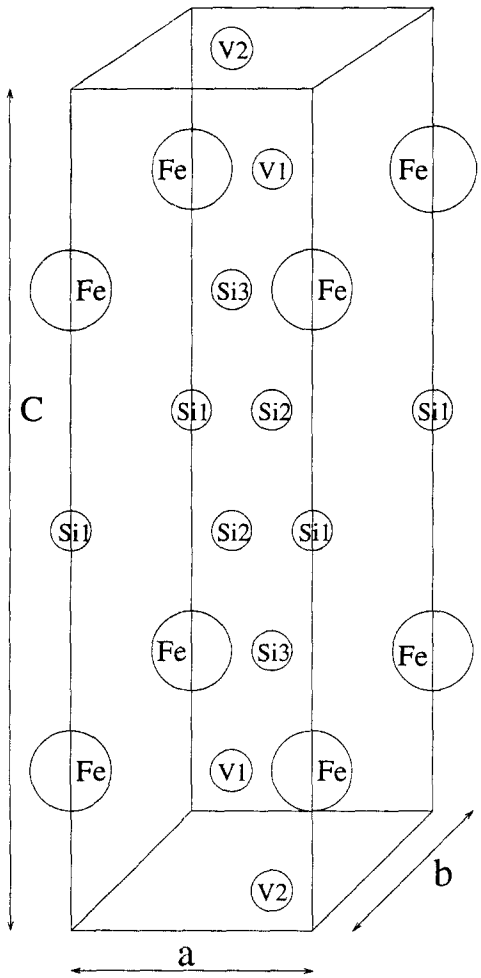

Fig. 1 The hexagonal unit cell of $Fe_1/Si_5/Fe_1$. The number of *Si* layers between *Fe* layers is five which are composed of two layers of *Si*3 and two layers of *Si*2 and one layer of *Si*1. In addition to two *Fe* and five *Si* layers, two vacuum layers are added to each *Fe* layer.

magnetic moments in surface and interface layers are examined with increasing the number of spacer layers.

2. Computational Methods

We have performed self-consistent LMTO electronic band structure calculations for a cubic B_2 phase of *FeSi* and for a series of $Fe_m/Si_n/Fe_m$ for $m = 1$, 3 and $n = 1$, 3, ···, 13, systematically. A supercell of the $Fe_m/Si_n/Fe_m$ sandwich with vacuum layers is considered to simulate the experimental system. We have used space-filling atomic spheres of equal size for both *Fe* and *Si* sites, and vacuum layers are treated as empty spheres in the LMTO band calculation. *s*, *p*, and *d*-state are included in the basis set for each site. We calculated density of states (DOS) by the tetrahedron method over 80 K points in the irreducible part of the Brillouin zone. For the electron-electron exchange-correlation, the von Barth-Hedin form has been utilized in the local spin density functional approximation.

The atomic geometry of $Fe/Si_5/Fe$ in Fig. 1 indicates that the lattice constance a in the $x-y$ plane is the same as that of *FeSi* (111) ($\sqrt{2}\,a_0$, ($a_0 = 2.717$ Å)), but the c value in the z-direction is determined from the number of layers N including vacuum layers ($\sqrt{3}\,a_0 N/6$). In trilayer calculations, we assumed 4-6 vacuum layers in order to isolate the system, and the number of vacuum layers is chosen to make calculations efficient for the trilayer.

3. Results and discussions

Using the lattice constant of B_2 phase reported by Kanel *et al.* [10], we have calculated the electronic structure of *FeSi* which corresponds to *CsCl* structure. The stable solution is paramagnetic. Fig. 2 presents DOS in the ground state paramagnetic phase, which has 0.05 *eV* band gap. One can see a rather broad band (~ 13 *eV* width) with strongly mixed *Fe* and *Si* states. This strong hybridization induces *Fe* to lose the magnetic moment. The present result is quite close to results of previous LDA calculations [13].

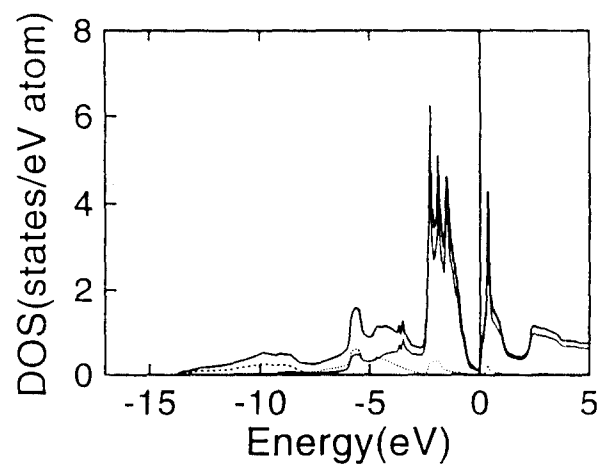

Fig. 2 Density of states of *FeSi*. The Fermi energy E_F corresponds to the zero of energy. Bold solid line represents the total DOS, and solid line represents the partial *d*-band of *Fe*, and dotted and dashed lines represent partial *s* and *p*-band of *Si*, respectively. The states near E_F are almost from the *Fe d*-band.

Next, we have calculated electronic structures for $Fe/Si_n/Fe$ trilayers which are grown along *FeSi* (111) direction (z-direction). In our calculation, no interface diffusion is assumed, and therefore *Si* spacer layer maintains the bcc structure. In Fig. 3, we show the band structure of trilayers near E_F with varying the number of spacer layers. One can easily notice that the states along the $\Gamma - A$ direction, which is parallel to the z-direction, do not disperse much, reflecting a two-dimensional nature of the *Fe/Si/Fe* trilayers. It is also found that a pair of localized states (denoted by *S*) near E_F move up across E_F with increasing two spacer layers. Every time the spacer layer increases, a new

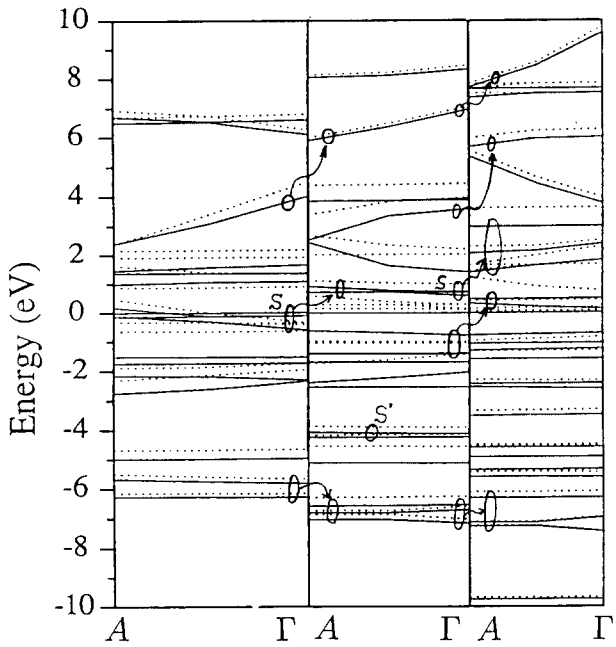

Fig. 3 The band structure of $Fe_1/Si_n/Fe_1$ along the $\Gamma - A$ direction which is parallel to the growth direction. The left panel is for $n = 3$, and the center and the right are for $n = 5$ and $n = 7$, respectively. The zero of energy is set to the Fermi energy. Almost all the states near and below E_F are rather flat reflecting a two-dimensional nature.

state (denoted by S') appears. In this study, band characters are determined by examining the site and angular momentum composition and the symmetry of each band.

In Fig. 4, DOS of $Fe_3/Si_5/Fe_3$ is plotted. DOS's in top three panels correspond to d-band DOS's of surface *Fe* (*Fe (S)*), center *Fe* (*Fe (C)*), and interface *Fe* (*Fe (I)*), respectively. It is seen that the bandwidth is narrow at the surface and becomes broad at the interface. Narrow band at the surface arises from the surface localization effect, while broad band at the interface originates from the hybridization effect between *Fe* and *Si* states. Sharp peak structures above the Fermi energy E_F in the minority spin bands move down in energy as going from the surface to the interface, revealing that *Fe* and *Si* hybridization occurs. The occupied d-electrons increase from the surface to the interface layer (6.4, 6.7, 7.0) due to the charge transfer, and thus more electrons fill up the minority spin band at the interface. Furthermore, the number of electrons in the majority spin band decreases at the interface, since the exchange splitting is reduced due to the hybridization effect. Therefore the magnetic moment becomes reduced at the interface.

Most notable in Fig. 4 is the fact that the spacer layer in *Fe*/Si_n/*Fe* is metallic, different from the common expectation. As a consequence, it is likely that the interlayer coupling in *Fe*/*Si* has the same origin as in metallic multilayers such as *Fe*/*Cr*. In contrast to the bulk *Si* which has no local moment, the spacer *Si* layers in *Fe*/Si_n/*Fe* are slightly spin polarized antiferromagnetically due to the molecular field arising from adjacent *Fe*

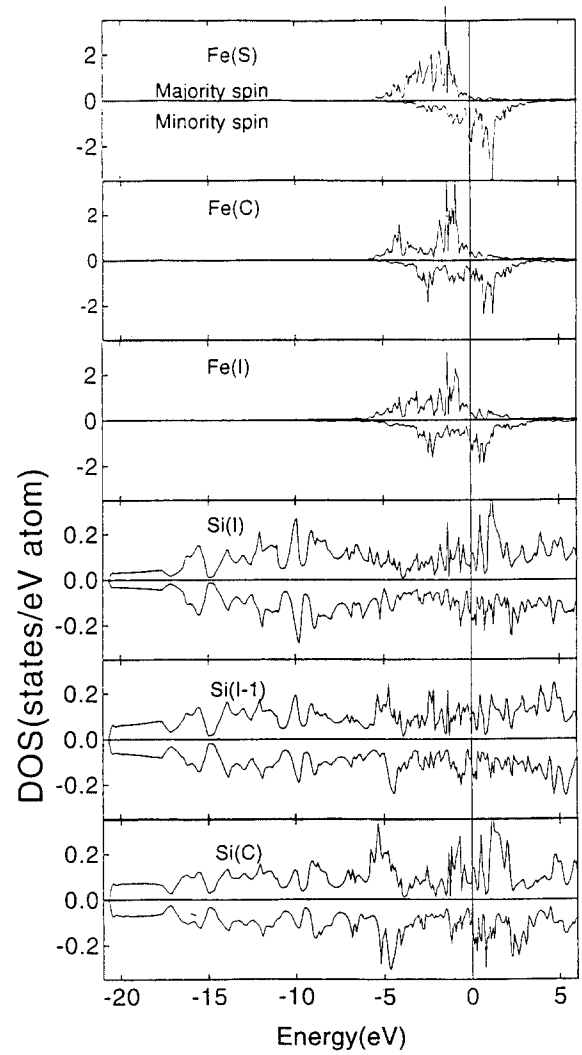

Fig. 4 Layer projected DOS for $Fe_3/Si_5/Fe_3$. Top three panels provide DOS's of the *Fe* 3d-band in surface (S), center (C), and interfacial (I) layer, respectively. Bottom panels provide DOS's of the spacer layer *Si* atoms.

layers. The calculated magnetic moment distributions in $Fe_3/Si_5/Fe_3$ layer have the following features. (i) For given ferromagnetic *Fe* layers, magnetic moments of *Si* spacer layers are antiferromagnetically oscillating with $0.02 - 0.04\ \mu_B$, and the size of magnetic moment is not dependent on the number of spacer layers. (ii) Magnetic moments of *Fe* atoms in surface, central and interfacial layers of $Fe_3/Si_5/Fe_3$ are 2.82 μ_B, 2.19 μ_B and 1.57 μ_B, respectively. The magnetic moment in the surface layer is much enhanced due to the surface localization effect, whereas the magnetic moment in the interfacial layer is much reduced due to the hybridization effect. The magnetic moment in the central layer is more or less the same as the bulk value. (iii) The coupling between interfacial *Fe* and *Si* is antiparallel.

Because of the strong *Fe* – *Si* hybridization, the magnetic moment per *Fe* atom in *Fe*/Si_n/*Fe* is reduced much as com-

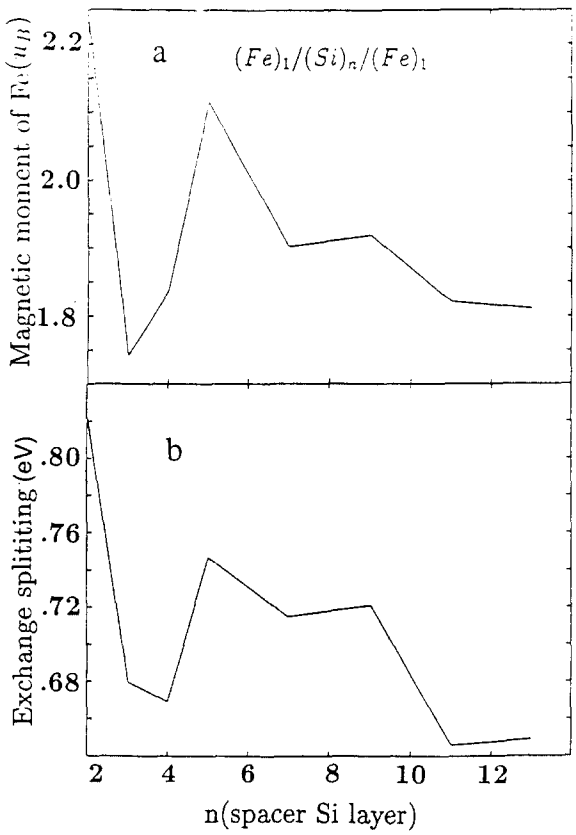

Fig. 5 The magnetic moment and the exchange splitting with varying the spacer layer thickness. Both quantities show the periodicity of 4 ML with an oscillatory decaying behavior.

pared to that of bulk Fe. As shown in Fig. 5(a), the magnetic moment per *Fe* in $Fe/Si_3/Fe$ trilayer is 1.75 μ_B which is ~80 % of bulk value. The magnetic moment in Fig. 5(a) and the ferromagnetic exchange splitting in Fig. 5(b) oscillate and decrease in magnitude with increasing the spacer layer thickness. This result is in good agreement with that of Jones *et al.* [7], which shows the oscillatory decaying behavior of the interlayer coupling. It is apparent that the magnetic moment and the exchange splitting has a periodicity of about 4 ML, as seen in Fig. 5.

To understand the mechanism that mediates the magnetic coupling between the ferromagnetic layers, we consider the Fermi surface of the *Si* spacer layer. The Fermi surface of *Si* spacer layer with B_2 phase is provided in Fig. 6. There are two Fermi wave vectors along $\Gamma - P$ line, long $k_F(1)$ and short k_F (2), which is parallel to the growth direction. The period in monolayers correspondings to the inverse of the distance between the Fermi wave vector and the Brillouin zone boundary wave vector(k_{ZB}), measured in unit of k_{ZB}. Using $k_{ZB} = \pi/d$ where d is the layer spacing, we arrive at the desired relation: period $/d = k_{ZB}/k_F$. Therefore the short wave vector $k_F(2)$ gives rise to a long period of 8 ML (monolayers), which is compatible with the observation [2]. Meanwhile, the longer Fermi

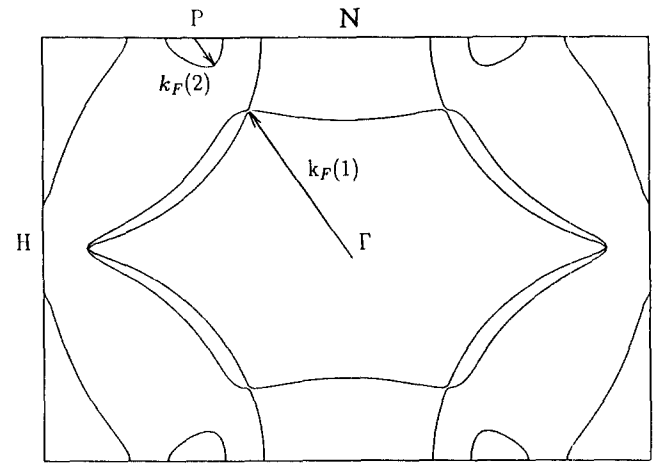

Fig. 6 The Fermi surface of bcc *Si*. There are two Fermi wave vectors along $\Gamma - P$ direction, which is parallel to the growth direction. One can obtain two different oscillatory periodicities from these wave vectors.

wave vector $k_F(1)$ yields a short period of 1.7 ML.

4. Conclusion

Electronic and magnetic properties of bulk *Fe/Si* and *Fe/Si/Fe* trilayer are studied. For bulk *Fe/Si*, we have obtained paramagnetic and insulating phase in agreement with previous results. In *Fe/Si*, *Fe* and *Si* band states are strongly mixed with a broad bandwidth, and so the *Fe* atom lose the magnetic moment.

From the study of band structures of *Fe/Si/Fe* varying the thickness of the spacer layer, We have found that the band states along the $\Gamma - A$ direction, which corresponds to the growth direction, do not disperse much reflecting a two-dimensional nature. It is also found that a pair of localized states near E_F move up across E_F with increasing every two spacer layers. DOS of the *Fe* surface layer in $Fe_3/Si_5/Fe_3$ well represents the surface localization effect, whereas that in the interfacial *Fe* layer is much delocalized due to the hybridization effect between interfacing atoms.

Overall amplitudes of the magnetic moment and the ferromagnetic exchange splitting decreases with increasing the thickness of spacer layers, and show the periodicity of ~4 ML. A short Fermi wave vector of bcc *Si* gives rise to a magnetic coupling period of ~8 ML. The spacer layer in the $Fe/Si_n/Fe$ is metallic, and thus the interlayer coupling in $Fe/Si_n/Fe$ seems to have the same origin as in metallic multilayers.

Acknowledgements

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