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Structure and magnetic properties of Fe4/Cun ($n = 2,4$) superlattices from first-principles study

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ABSTRACT

The structures and magnetic properties of Fe4/Cun ($n = 2, 4$) superlattices have been investigated by the first-principles pseudopotential plane-wave method based on spin density approximation. Compared with the ideal fcc-Cu bulk structure, for the optimized Fe4/Cu2 model, obvious contraction of interlayer distances occurs on the interior Fe layers, whereas the interlayer distances of Fe layers in Fe4/Cu4 are expanded. The anti-parallel alignment magnetic moment and negative polarization of the interior Fe layer have been found in the Fe4/Cu2 model. This can be explained in terms of the magnetic-volume effect, and the moment of anti-parallel alignment attributes to the contracted interlayer distances between the interior Fe layers. The MR ratio has also been evaluated by means of the two-current model. The MR ratio of the Fe4/Cu2 model (4.89%) is much small than that of the Fe4/Cu4 one (23.65%).

1. Introduction

The electronic and magnetic properties, especially giant magnetoresistance (GMR) effect [1] of the fcc-Fe/Cu system, have been the subjects of great interest for many years because of its wide application potential in magnetic storages. The GMR [2,3] effect in a magnetic layered structure is induced by an asymmetry in scattering rates for up- and down-spin electrons (the so-called spin-dependent scattering). Most theories recognize the spin-dependent scattering at the interface as the main origin for the GMR effect. However, the spin-dependent scattering in bulk cannot be neglected, and the electronic structure and properties of the magnetic layer are also the key factors for the GMR effect.

The magnetic property of the fcc-Fe/Cu system has been the subject of an enormous number of experimental as well as theoretical studies. Series fcc-Fe/Cu (0 0 1) superlattices were prepared by the epitaxial growth of fcc-Fe on Cu (1 0 0) layers experimentally by Mitani et al. [4] to study the correlation of magnetic moment versus interlayer distance. The prepared fcc-Fe exhibited various magnetic properties, from collinear ferromagnetism (FM), antiferromagnetism (AF), or bilayer antiferromagnetism (bilayer AFM), to a spiral spin structure [5], which also attracted much attention for theoretical investigations. The magnetic properties and structure of the Fe/Cu (1 0 0) surface and Cu/Fe(n)/Cu sandwich system had been studied extensively by first-principles calculations [6,7]. Only a few attempts had been made to study the magnetic properties of the Fe/Cu superlattice. The total energy as a function of collinear spin configurations and Fe layer thickness for Fen/Cu (0 0 1) ($n = 1$–9 ML) superlattices [8] had been calculated. But most of the calculations were performed for the ideal fcc structure, and no relaxation of the interlayer distance was considered. The researches confirm the ferromagnetic character of the film with up to 3 monolayer (ML) Fe and show that the observed tetragonal distortion [9] is due to the expanded volume of the FM high-spin state. Films with more than 4 ML assume various AF configurations, even non-linear configurations. However, dispute still exists between theory and experiment concerns on the transition regime of the 4 ML Fe system: theory predicts as a kind of AF coupling, FM ordering is reported by experiment. Little attention has been paid to the effect of electronic structure and magnetic coupling (AF or FM) in the Fe layers on the GMR effect. In this paper, we carry out the first-principles calculations for the magnetic properties and electronic structure of the Fe4/Cun ($n = 2$, 4) superlattices. We focus our attention on the delicate correlation between the structure and magnetic properties of this system, and also provide some understandings of the dependence of GMR on the electronic structure and the magnetic phase of Fe layers.

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2. Computational method and models

In our calculation, the structure and magnetic properties of fcc-Fe/Cu (1 0 0) superlattices have been investigated. The fcc-based superlattices consisting of 4 atomic layers of Fe and n ($n = 2, 4$), atomic layers of Cu are constructed stacking along the [1 0 0] direction by adopting the lattice constant of bulk Cu as shown in Fig. 1. The models are labeled from the bottom of the Fe layers, so Fe1, Fe2, Fe3, and Fe4 represent the first, second, third, and fourth layers of Fe, respectively; the Cu1 is numbered as the fifth layer, and so on. We perform first-principles calculations within the density functional theory (DFT) [10] using the Cambridge Serial Total Energy Package (CASTEP) code. The exchange and correlation potential is described by Perdew and Zunger parameterization [11], the plane-wave cutoff energy is set at 280.0 eV. The number of sample k point is $8 \times 8 \times 2$. Geometry optimization is carried out until the force of each atom is less than 0.05 eV/Å.

3. Results and discussion

The change ratios of the interlayer distance of optimized models are presented in Fig. 2. The Fe/Cu interfaces are marked by arrows. For the Fe/Cu interface, there are no obvious changes of interlayer spacing except for d45 in the Fe4/Cu2 model. In the Fe4/Cu2 model, the interlayer distances of the Fe layers (except d34) contract, and the interlayer distances between the Fe2 layer with the neighboring layers contract as high as 5%. Moreover, the interlayer distance is expanded 4% in the interior Fe layers in the Fe4/Cu4 model. As noted by investigation [12,13], for metastable fcc-Fe on Cu (1 0 0), about 5% variation of the interlayer distance that is compatible with subtle structural differences of the Fe phase on Cu (1 0 0) is enough to switch among the various magnetic phases. The delicate correlation between the interlayer distance and the magnetic moment will be discussed in the following section.

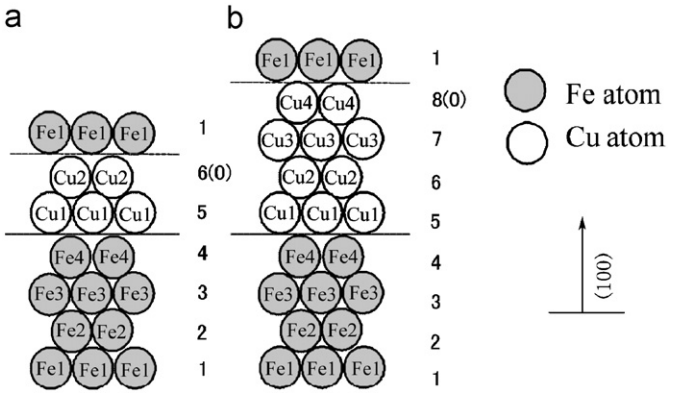

Fig. 1. The sketch of Fe4/Cu2 and Fe4/Cu4: (a) Fe4/Cu2 and (b) Fe4/Cu4.

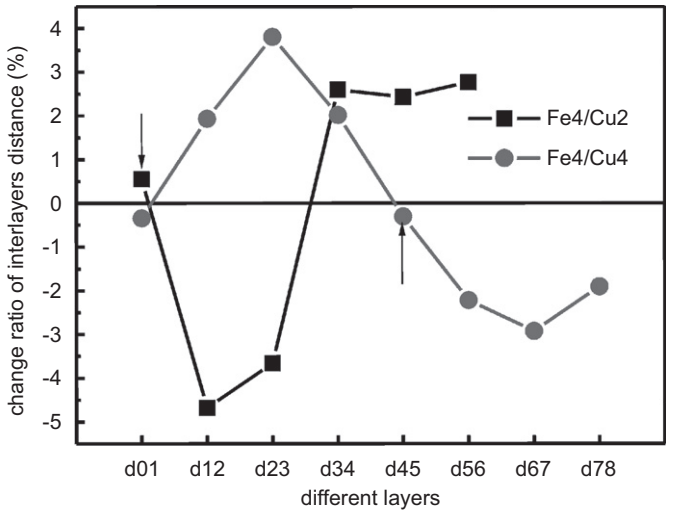

Fig. 2. The change ratios of the interlayer distance of the Fe4/Cu2 and Fe4/Cu4 models compared with the bulk Cu interlayer distance. d01 and d45 represent the interface distance, which are marked by arrows; d12, d23 and d34 represent the Fe interlayer distances d56, d67, d78 represent the Cu interlayer distances, respectively. The positive and negative represent the expansion and contraction of the interlayer distance, respectively.

The magnetic moment and charges are obtained by Mulliken population analysis [14]. We can see that for Fe4/Cu2 and Fe4/Cu4 models, the charge transfer occurs primarily at the Fe/Cu interface, whereas very little charge transfer is observed in the interior layers of Fe and Cu. The net charges transfer from the Fe to the Cu atoms. The interface Fe layers lose 0.21 electrons and the interface Cu layers gain 0.23 electrons (0.22 electrons). The charge transfer behavior is contributed to the relative positions of the Fermi levels, and because bulk Cu has a lower Fermi energy than that of bulk γ-Fe [15].

When it comes to the magnetic moment, there exist significant differences between Fe4/Cu2 and Fe4/Cu4. As shown in Table 1, the magnetic moment of Fe2 is $-2.18\ \mu_B$ (the minus represents the opposite magnetic ordering with neighboring layers), which means the antiferromagnetic phase exists in the magnetic Fe layers for the Fe4/Cu2 model. For the Fe4/Cu2 model, referring to Fig. 2, through the analysis of interlay distance and magnetic moment, the main contraction comes from the interior Fe layer, which has the opposite magnetic moment. On the other hand, for Fe4/Cu4, the expansion of the Fe interlayer distances (atomic volume of Fe) results in the high-ferromagnetic state. The magnetic moment for the Fe layers is all above $2.6\ \mu_B$ (2.6–$2.78\ \mu_B$). This consists with the magnetic-volume effect [16], which describes the relationship between the interlayer distance and the magnetic coupling. Referring back to our former research on Fe3Cux ($x = 3, 5$), the interlayer distances of Fe layers in Fe3Cu3 and Fe3Cu5 are all expanded, and the magnetic moments for the Fe layers are all above $2.6\ \mu_B$ (2.6–$2.78\ \mu_B$), which is called the high-ferromagnetic state. The results consist with the experimental and other theoretical results [4,13]. As shown by our research, in fact the changes of Cu layer thickness in Fe3Cux models have not caused obvious differences of the magnetic state between Fe3Cu3 and Fe3Cu5. Being different from the Fe3Cux system, the magnetic states of the fcc-Fe/Cu systems containing 4 Fe layers are really complex and delicate, and the change in the number of nonmagnetic Cu ML affects the arrangement of

Table 1
The magnetic moment and charges of different atom layers for Fe4/Cu2 and Fe4/Cu4 models

	Models	Atom layer							
		Fe1	Fe2	Fe3	Fe4	Cu1	Cu2	Cu3	Cu4
Charge (e)	Fe4/Cu2	0.20	0.02	0	0.19	−0.21	−0.20		
	Fe4/Cu4	0.21	−0.02	−0.02	0.21	−0.22	0.03	0.03	−0.22
Magnetic moment (μ_B)	Fe4/Cu2	2.42	−2.18	2.40	2.70	−0.06	−0.04		
	Fe4/Cu4	2.78	2.60	2.60	2.78	−0.02	0.04	0.04	−0.02