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Retraction

Electronic structures and magnetism of Fe nanowires on Cu(001) and Ag(001): A first-principles study
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Announcement of Editorial Office of Chinese Physics. Due to the fault of the author(s), the article entitled "Electronic structures and magnetism of Fe nanowires on Cu(001) and Ag(001): A first-principles study", published in 2007 Vol.16, No.2, pp506-510, has been clarified to be a duplicate of the following articles, which have been published in (i) Jin Y J et al 2004 *Physica Status Solidi* b241 pp1431-1434; (ii) Jin Y J et al 2005 *Journal of the Korean Magnetics Society* Vol.15 pp217-220. So the above article in Chinese Physics will be withdrawn from the publication.

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Electronic structures and magnetism of Fe nanowires on Cu(001) and Ag(001): A first-principles study*

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The electronic structures and magnetism of Fe nanowires along the [110] direction on Cu(001) and Ag(001) [Fe(nw)/Cu(001) and Fe(nw)/Ag(001)] are investigated by using the all-electron full-potential linearized augmented plane wave method in the generalized gradient approximation. It is found that the magnetic moment of Fe atom for the Fe(nw)/Cu(001) is 2.99 μ_B, which is slightly smaller than that (3.02 μ_B) for the Fe(nw)/Ag(001) but much larger than that (2.22 μ_B) for the bcc iron. The great enhancement of magnetic moment in the Fe nanowires can be explained by the Fe d-band narrowing and enhancement of the spin-splitting due to a reduction in coordination number. From the calculated spin-polarized layer-projected density of states, it is found that the Fe 3d-states are strongly hybridized with the adjacent Cu 3d-states in the Fe(nw)/Cu(001), and there exists a strong hybridization between the Fe sp- and the adjacent Ag 4d-states in the Fe(nw)/Ag(001).

Keywords: nanowire, electronic structure, magnetism, full-potential linearized augmented plane wave

PACC: 7115A, 7120H

1. Introduction

Nanowire is one of the important building blocks in the nano-electronic devices. Especially, magnetic nanowires have attracted much attention due to their potential applications in high-density memory storage devices. Recently, the cylindrical shape nanowires with diameters ranging from 20 to 500 nm and lengths of about 10 μm have been synthesized by the template-directed and the thermal evaporation methods.[1−5] Such nanowires can be applied to perpendicular magnetic recording media. Another important method of synthesizing magnetic nanowires is the growth of nanowires on a suitable substrate, for example, Co chains on a Pt(997) surface[6] and Fe stripes on a vicinal W(110) surface.[7] The copper is an excellent substrate for the growth of Fe thin films[8] due to the small mismatch of the lattice constant between the fcc copper (3.61 Å) and the metastable fcc iron (3.59 Å). Shen *et al*[9] produced quasi-one-dimensional Fe stripes with a height of 1–2 atomic diameters and width of 5–15 atomic diameters, on a stepped Cu(111) surface by using a step-edge decoration.

The fabrications of the nanowires with a diameter of one atom are not available based on the present technology. However, some theoretical work exists on the nanowires,[10,12−16] which will give some comprehensive insight into the fundamental properties of the nanowires. Previously, Weinert and Freeman[10] have used self-consistent full-potential linearized augmented plane wave (FLAPW)[11] band calculation method to predict that the free standing linear chains of Fe and Ni would be 'strong' stoner ferromagnets with large magnetic moments (3.3 μ_B for Fe and 1.1 μ_B for Ni) and large s- and d-exchange splittings. Recently, Yang *et al*[12] have investigated three types of nanowire systems, i.e. Fe atomic chain, fcc Fe nanowire, and bcc Fe nanowires by using the FLAPW method. They found great enhancements in the spin magnetic moments of 3.30, 3.02, and 3.06 μ_B/atom for the Fe chain, the bcc Fe nanowire, and the fcc Fe nanowire, respectively. Those results indicate that the reduced dimensionality and the reduced coordination number are responsible for the dramatic enhancement in magnetic moments. Spišák *et al*[13] have investigated the position dependence of the magnetic moment of Fe nanowires on a high-index surface of Cu(117) by using a pseudopotential method. They

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considered six different locations of the Fe nanowire and found the inner corner site of the Cu(117) step to be the most stable position with a magnetic moment of $2.80\,\mu_B$/atom but the top of the terrace of the vicinal Cu(117) to be the most unstable position with a magnetic moment of $2.96\,\mu_B$/atom. Previously, we[14] have investigated the electronic structures and magnetism of the Fe nanowire along the [010] direction on Cu(001) (Fe[010] nanowire) by using the FLAPW method. We found that the Fe magnetic moments were enhanced to 3.11 and $3.39\,\mu_B$/atom for the Fe[010] nanowire and the free-standing Fe nanowire, respectively.

In this paper, in order to understand the effects of different substrates on the electronic structures and magnetism of the Fe nanowires, we perform the first-principles calculations by using the highly precise all-electron FLAPW method in the generalized gradient approximation (GGA).[17] In Section 2, we briefly describe the calculational model and method. The results and discussion are presented in Section 3. Finally, a brief summary is given in Section 4.

2. Calculational Method

The Fe nanowires along the [110] direction separately on Cu(001) and Ag(001) [denoted by Fe(nw)/Cu(001) and Fe(nw)/Ag(001)] respectively are modelled by an Fe nanowire attached to each side of a five-layer-thick Cu(001) slab and an Ag(001) single slab as illustrated in Fig.1. The two-dimensional (2D) unit cells are chosen to be of p(3×1) structure. Along the y-axis, the 2D lattice constants are set as 4.83 and 5.47 a.u.[18] for the Fe(nw)/Cu(001) and the Fe(nw)/Ag(001), respectively. The spacings between the Fe nanowire and the Cu and Ag substrates are assumed to be 3.41 and 2.67 a.u., respectively, those are evaluated by keeping the atomic volume of the iron the same as that of the bcc iron. Neither surface relaxation nor reconstruction is considered.

The Kohn–Sham equation[19] has been solved self-consistently by using the FLAPW method in the GGA of an exchange-correlation potential. Lattice harmonics with $l \leq 8$ are employed to expand the charge density, potential, and wavefunctions within the muffin-tin (MT) radii of 2.2 and 2.4 a.u. for the Fe(and Cu) and Ag atoms, respectively. An energy cut-off of 13 Ry is employed for the basis set and a 210-Ry star function cut-off is used for depicting the charge density and potential in the interstitial region. Integrations inside the 2D Brillouin zone (BZ) are replaced by summations over a 6×18 mesh corresponding to $27\,\boldsymbol{k}$ points inside the irreducible 1/4 wedge of the 2D BZ. All core electrons are treated fully relativistically while valence states are treated scalar relativistically, i.e. without spin-orbit coupling.[20] Self-consistency is assumed when the difference between the input and the output charge (spin) densities is less than 1.0×10^{-4} electrons/(a.u.)^3

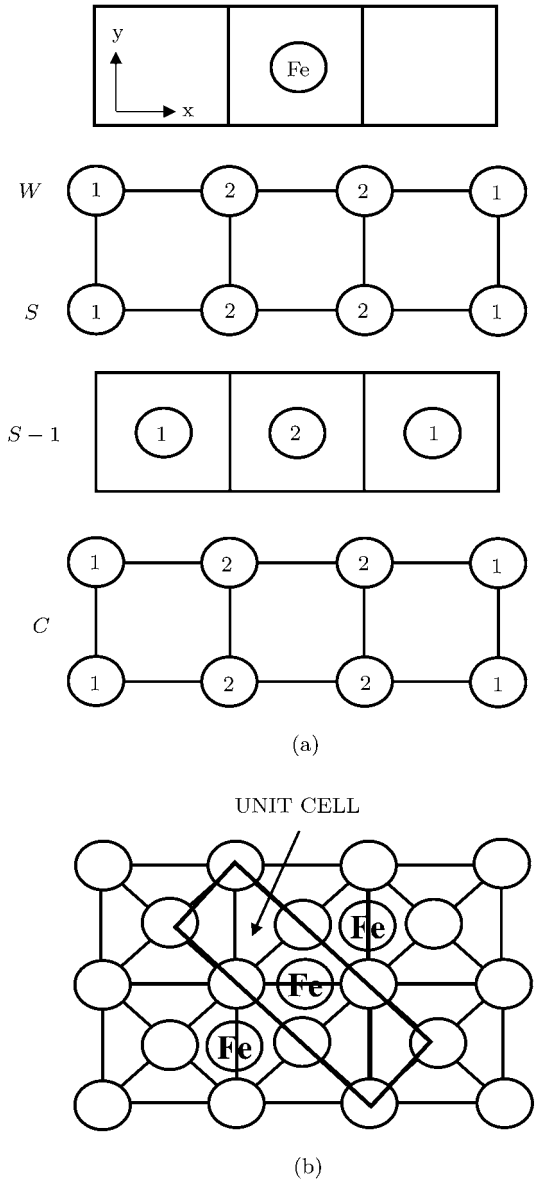


Fig.1. Schematic representations for (a) side view and (b) top view of the Fe nanowire on Cu or Ag(001) surfaces. Labels W, S, $S-1$, and C represent the chain, the surface, the subsurface, and the central layers, respectively. In each layer, the numbers in the circles represent distinct atomic sites from the symmetry point of view.

3. Results and Discussion

The spin-density contour plots for the Fe(nw)/Cu(001) and the Fe(nw)/Ag(001) in the (310) plane are presented in Fig.2. The solid and the broken lines represent positively and negatively polarized spin densities, respectively. The lowest contour starts from $\pm 5 \times 10^{-4}$ electrons/(a.u.)^3, and the subsequent lines differ by a factor of $\sqrt{2}$. Overall shapes of the spin densities are very similar in the two systems and they are similar to the shape of spin density in the clean bcc Fe(001) surface.[21] There exist large eruptions of the majority spins from the Fe atoms toward the vacuum region, which indicates the large enhancement in magnetic moment of the Fe atoms. We can see that the nearest neighbour (n.n.) Cu (or Ag) atoms of the Fe atom are slightly positively spin-polarized but negatively spin-polarized in the interstitial regions between the Fe and the adjacent Cu(or Ag) atoms, while the spin-polarizations of other Cu (or Ag) atoms are negligible.

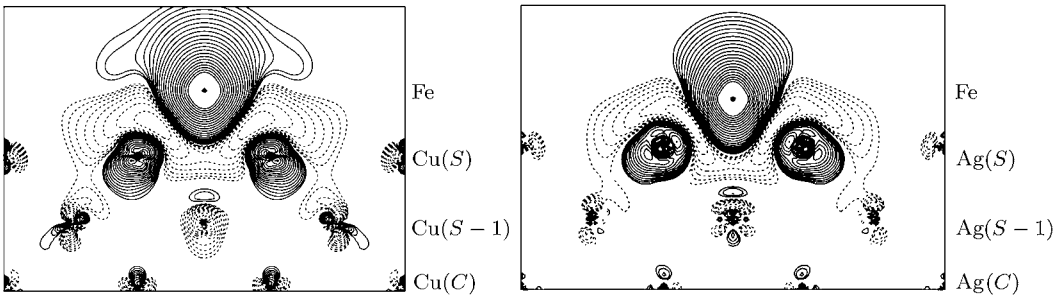


Fig.2. Spin density contour plots of (a) the Fe(nw)/Cu(001) and (b) the Fe(nw)/Ag(001) in the (310) plane. The solid and the broken lines represent positively and negatively polarized spin densities, respectively. The lowest contour starts from $\pm 5 \times 10^{-4}$ electrons/(a.u.)^3, and the subsequent lines differ by a factor of $\sqrt{2}$.

Table 1. The l-decomposed majority and minority spin electrons of Fe atoms in the MT spheres, the magnetic moments of Fe atoms (in units of μ_B), the numbers of n.n. atoms, the Fe–Fe bond lengths, and the Fe-(Cu or Ag) bond lengths for the Fe(nw)/Cu(001), the Fe(nw)/Ag(001) and the free-Fe(nw)s.

system	spins	s	p	d	M	n.n.	Fe–Fe	Fe-(Cu or Ag)
Fe(nw)/Cu(001)	↑	0.18	0.08	4.44	2.99	6	4.83	4.83
	↓	0.15	0.07	1.49				
	total	0.33	0.15	5.93				
Fe(nw)/Ag(001)	↑	0.18	0.09	4.47	3.02	4	5.47	4.70
	↓	0.15	0.08	1.49				
	total	0.33	0.17	5.96				
free-Fe(nw)[22]	↑	0.20	0.04	4.52	3.20	2	4.83	-
	↓	0.15	0.03	1.39				
	total	0.35	0.06	5.91				
free-Fe(nw)[14]	↑	0.21	0.01	4.59	3.39	2	6.83	-
	↓	0.13	0.01	1.28				
	total	0.34	0.01	5.87				

The l-decomposed majority and minority spin electrons of Fe atoms inside the MT spheres, the magnetic moments of Fe atoms (in units of μ_B), the numbers of n.n. atoms, the Fe–Fe bond lengths, and the Fe-(Cu or Ag) bond lengths for the Fe(nw)/Cu(001) and the Fe(nw)/Ag(001) are given in Table 1. For comparison, those for the free standing Fe nanowires (free-Fe(nw)s) are also given in Table 1. The Fe magnetic moment of the Fe(nw)/Cu(001) is 2.99 μ_B/atom that is slightly smaller than that (3.02 μ_B/atom) of the Fe(nw)/Ag(001) but 35% larger than that (2.22 μ_B/atom) of the bcc iron. The free-Fe(nw) with the largest Fe–Fe bonding length has the largest magnetic moment of 3.39 μ_B/atom. As expected, the en-

hancement in Fe magnetic moment is closely related to a reduction in coordination number. The coordination number of Fe atoms decreases from 6 for the Fe(nw)/Cu(001) to 4 for the Fe(nw)/Ag(001) and to 2 for the free Fe(nw)s. It is found that the bond length of Fe–Fe atoms also affects the magnetic moment of Fe atom. The magnetic moments of Fe nanowires increase as the Fe–Fe bond lengths increase.

On the other hand, the n.n. Cu(Ag) atoms from the Fe atom have a small induced magnetic moment of $0.04\,\mu_{\mathrm{B}}$ ($0.03\,\mu_{\mathrm{B}}$), and the magnetic moments of other Cu atoms are almost zero. The feature indicates that the Cu and Ag substrates are rather inert to the external magnetic perturbation from the Fe chain.

In Table 1, we also present the numbers of the l-decomposed majority and minority spin electrons in an MT sphere for the various systems. It is found that the numbers of p-electrons in Fe atoms decrease significantly, which is due to the p-electrons spilling out into the vacuum region. On the other hand, the numbers of s- and d-electrons in Fe atoms in an MT sphere are kept nearly constant, their values are about 0.3 and 5.9, respectively. The magnetic moments of the Fe atoms almost all originate from the spin polarization of the localized d-electrons, while the contribution from the spin polarization of the s- and p-electrons are very small.

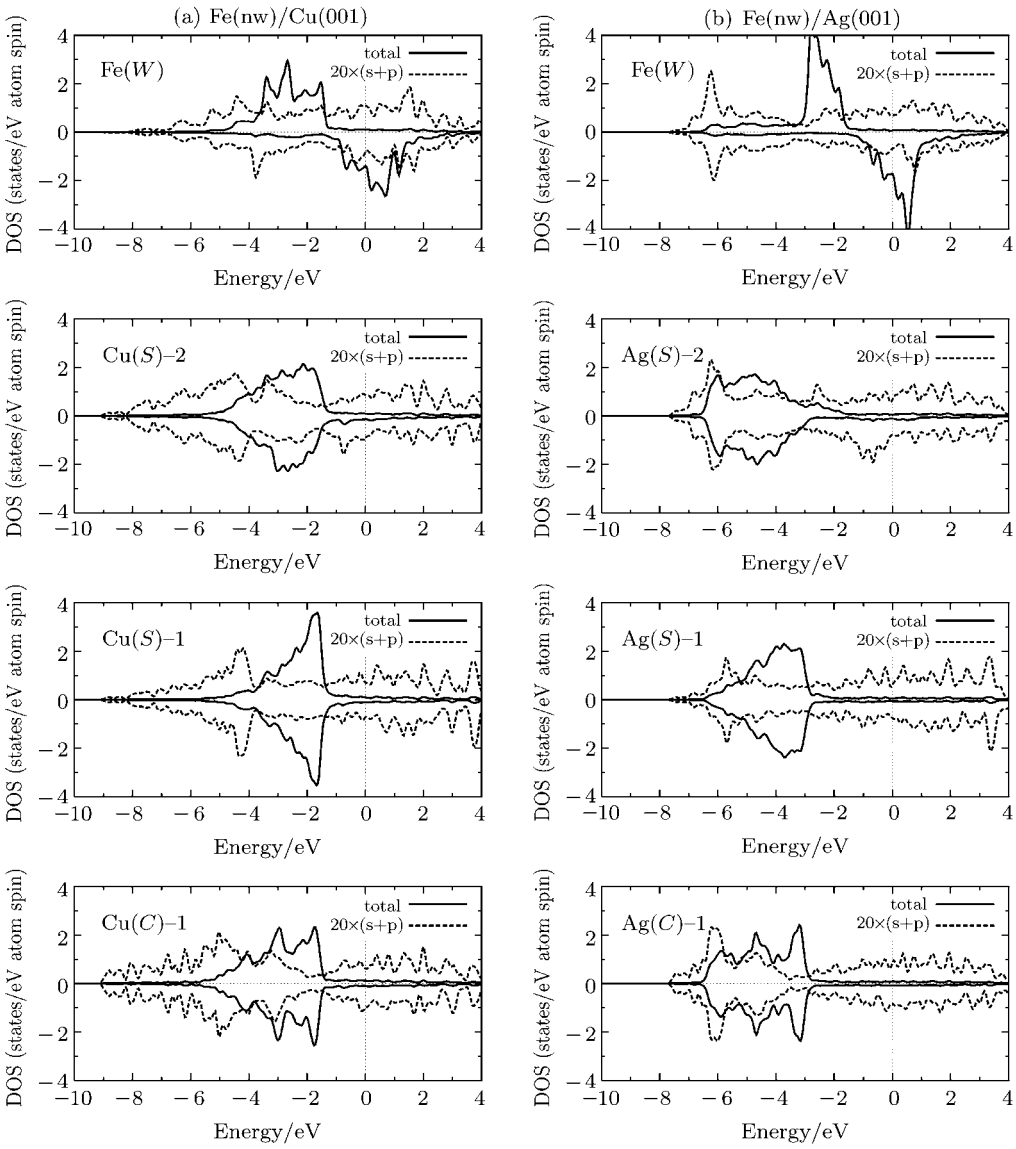


Fig.3. Spin-polarized layer-projected density of states (in units of states/eV atom spin) for (a) the Fe(nw)/Cu(001) and (b) the Fe(nw)/Ag(001). The minority spins are factored by -1, and the values of the sp states in the LDOS is multiplied by 20. The Fermi levels (E_{F}) are set to be zero.

The enhanced magnetic moments of the Fe nanowires can be understood from the calculated spin-polarized layer-projected density of states (LDOSs). The LDOSs for (a) the Fe(nw)/Cu(001) and (b) the Fe(nw)/Ag(001) are presented in Fig.3. The minority spins are factored by -1, and the values of the sp-states in the LDOS are factored by 20 for an easy comparison. The Fermi levels (E_F) are set to be zero.

As can be seen, the Fe d-bands for the Fe(nw)/Cu(001) and the Fe(nw)/Ag(001) are significantly localized compared with the bcc iron[23] due to a reduction in coordination number. For the Fe(nw)/Cu(001), the majority Fe 3d-bands are located from -4.5 to -1.3 eV and strongly hybridized with the majority 3d-bands of the nearest Cu atom. On the other hand, for the Fe(nw)/Ag(001) the majority Fe 3d-bands are positioned from -3.2 to -1.5 eV, while the 4d-bands of Ag(S)-2 atoms are located in a lower energy range from -6.5 to -3.0 eV. The strong hybridization between the Fe sp- and the nearest Ag 4d-states can be confirmed from the peaks of Fe sp-states at ~ -6.2 eV.

The reduction in coordination number also induces the great enhancement in spin splitting of Fe 3d-bands. The spin splitting of Fe atom for the Fe(nw)/Cu(001) is $\sim$ 2.9 eV that is much larger than that of the clean Fe(001) surface[21] or the bulk iron,[23] but it is slightly smaller than that ($\sim$ 3.2 eV) for the Fe(nw)/Ag(001). The fact is consistent with the result: the magnetic moment of Fe for the Fe(nw)/Ag(001) is larger than that for the Fe(nw)/Cu(001).

4. Summary

The electronic structures and magnetism for the Fe(nw)/Cu(001) and Fe(nw)/Ag(001) have been investigated by using the FLAPW method in the GGA of the exchange-correlation potential. The spin-density shows a large eruption of the majority spins from the Fe sites toward the vacuum region, which is consistent with the great enhancement in Fe magnetic moment. The calculated magnetic moment of Fe atom for the Fe(nw)/Cu(001) is 2.99 μ_B/atom that is slightly smaller than that (3.02 μ_B/atom) of the Fe(nw)/Ag(001), but about 35% larger than the magnetic moment (2.22 μ_B/atom) for the bcc iron. The largest magnetic moment of the Fe atom is found in the free-standing Fe(nw) with the largest Fe–Fe bond length. The great enhancement of magnetic moment in the Fe nanowires can be understood by the Fe d-band narrowing and enhancement of the spin-splitting due to a reduction in coordination number. The Fe–Fe bond lengths also affect the magnetic moments of the Fe nanowires that increase as the Fe–Fe bond lengths increase. The LDOSs show that the Fe 3d-states are strongly hybridized with the adjacent Cu 3d-states in the Fe(nw)/Cu(001), while there exists a strong hybridization between the Fe sp- and the adjacent Ag 4d-states in the Fe(nw)/Ag(001).

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