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First-principles-based study of transport properties of Fe thin films on Cu surfaces

Tomoya Kishi[1], **Hideaki Kasai**[1], **Hiroshi Nakanishi**[1], **Wilson Agerico Diño**[1,2,3] **and Fumio Komori**[4]

[1] Department of Applied Physics, Osaka University, Suita, Osaka 565-0871, Japan
[2] Japan Science and Technology Agency, Kawaguchi, Saitama 332-0012, Japan
[3] Physics Department, De La Salle University, Taft Avenue, 1004 Manila, Philippines
[4] Institute for Solid State Physics, University of Tokyo, Kashiwa, Chiba 277-8587, Japan

E-mail: kasai@dyn.ap.eng.osaka-u.ac.jp

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Abstract

We investigate the transport properties of Fe thin films on Cu(111) based on first principles calculation. We calculate the electron current through these Fe thin films, which can be observed by using a double-tipped scanning tunnelling microscope. We find that the conductance is majority spin polarized. On the basis of the band structures for this system, we discuss the origin of these interesting transport properties.

1. Introduction

Magnetic nanostructures, thin films, multilayers, atom bridges, and dots are finding ever increasing importance as materials to support today's information society [1–10]. In particular, Fe thin films on Cu surfaces are attracting much attention because of the exhibited dependence of the structures and magnetic properties on the film thickness [1]. On Cu(111), the ferromagnetic Fe thin film can be fabricated layer by layer with the laser molecular beam epitaxy technique [10]. In our earlier study based on the density functional theory [2, 3], we found that the distance between the Fe atoms and the Cu(111) is 2.16 Å, and that the magnetic moment of the Fe atom is 2.7 μ_B, which is larger than that of Fe bulk, 2.0 μ_B. In addition, we investigated the band structure of this system and found that there were some surface localized states as we found for the Fe nanowires [8].

The scanning tunnelling microscope (STM) has become a major tool for analysing the surface structure and electronic states. By using a double-tipped STM, it is possible to measure the transport properties through arbitrary nanostructures on surfaces. In this paper, we investigate the transport properties through these Fe thin films, which can be observed by using this double-tipped scanning tunnelling microscope [11]. In the next section, we present

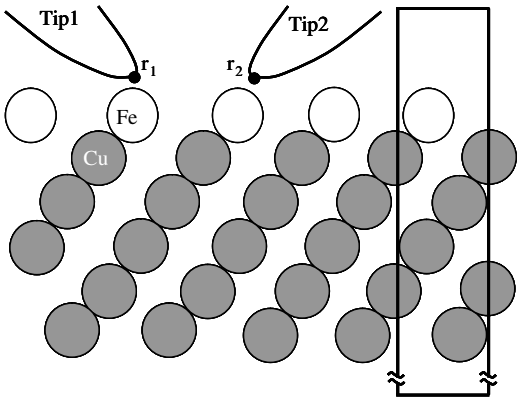

Figure 1. Side view of our model system. The position of the STM tip is $\mathbf{r}_i$. Grey circles indicate Cu atoms and white circles indicate Fe atoms. The rectangle indicates the super-cell for first principles calculation.

the computational details. In section 3, we show the numerical results. In the last section, we summarize the results.

2. Computational details

The system we consider in this study is shown in figure 1. The sample surface consists of one Fe layer and five Cu layers. The conductance of an electron from one tip (tip 1) to the other (tip 2), through the sample, can be accounted for by the Fermi golden rule [11], yielding

$$\sigma = \frac{2\pi e^2}{\hbar}\Gamma_1\Gamma_2\left|\sum_n \frac{\Psi_n(r_1)\Psi_n^*(r_2)}{\varepsilon_{\mathrm{F}} - \varepsilon_n}\right|^2, \tag{1}$$

where Ψ is the one-electron wavefunction and ε is the energy eigenvalue. Γ_i describes tip–sample coupling and is just a function with the period of the surface unit cell. We assume that the wavefunctions of the tips are represented by delta functions. The eigenvalues and wavefunctions are obtained by first principles calculations based on the density functional theory as follows. We use plane waves and ultrasoft pseudopotentials [12]. The plane-wave set is cut off at kinetic energies of 35 Ryd. We use 2353 k-points to sample the two-dimensional Brillouin zone. For the exchange–correlation energy, we adopted the generalized gradient approximation (GGA) [13]. All numerical results are obtained by spin-polarized GGA calculations with ferromagnetic initial configurations.

3. Results and discussion

We plot the conductance as a function of the distance between the tips as shown in figure 2. The position of tip 1 is fixed on the top site of the Fe atom and the position of tip 2 varied in the plane. The distance between each tip and the surface is 2.3 Å. In the case of both electron spins, the conductance decays as the distance between the tips increases. This is similar to the case of the Fe adatom on Cu(111) [14–18 and references therein]. The conductance for minority spin electrons decays much faster than that for majority spin electrons, so the electron current through the Fe thin film is majority spin polarized. Note that the oscillations observed in figure 2 do not reflect the atomic configuration, but are related to the direction-dependent

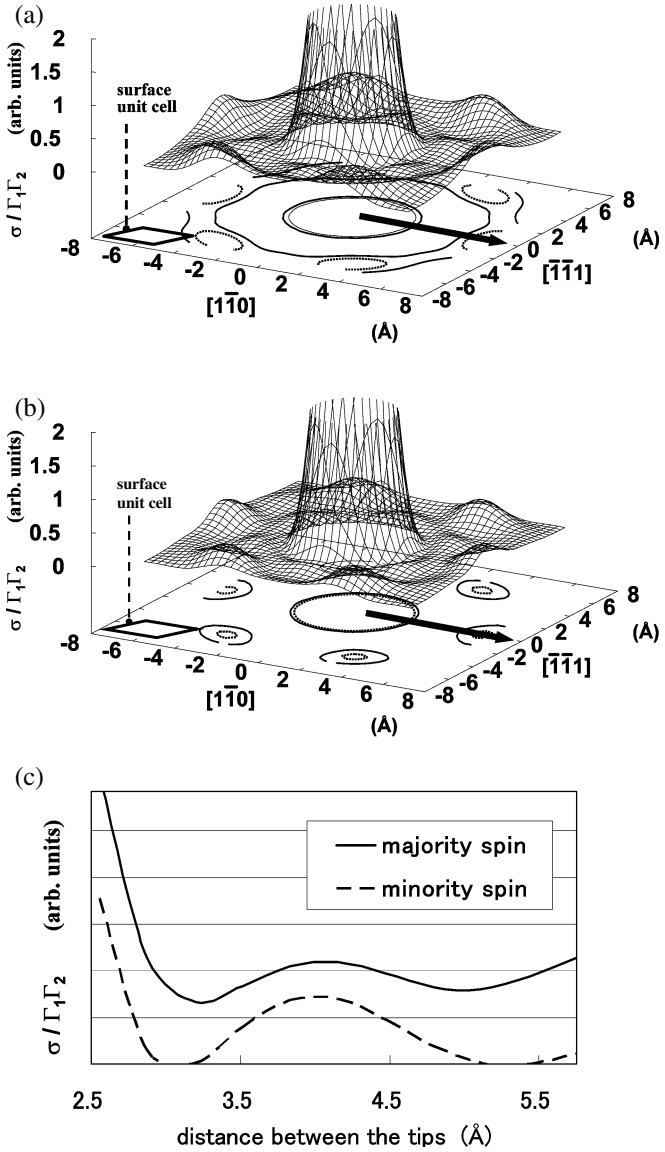

Figure 2. The distance and angular dependence of the conductance for (a) majority spin electrons and (b) minority spin electrons. (c) The corresponding conductance along the arrow lines shown in (a) and (b). The origin of the surface corresponds to the position of tip 1.

energy dispersion around the Fermi level. The corresponding band structures of the system are shown in figure 3. These bands have two-dimensional dispersion, so the conductance decays as mentioned above. The band dispersions differ greatly for each electron species. For example, the d bands for majority spin electrons lie between -4.0 and -2.0 eV as shown in [6]. On the other hand, those for minority spin electrons lie around the Fermi level. However, the difference in the conductance is slight. This is because there are no surface localized states across the Fermi level as shown in [3].

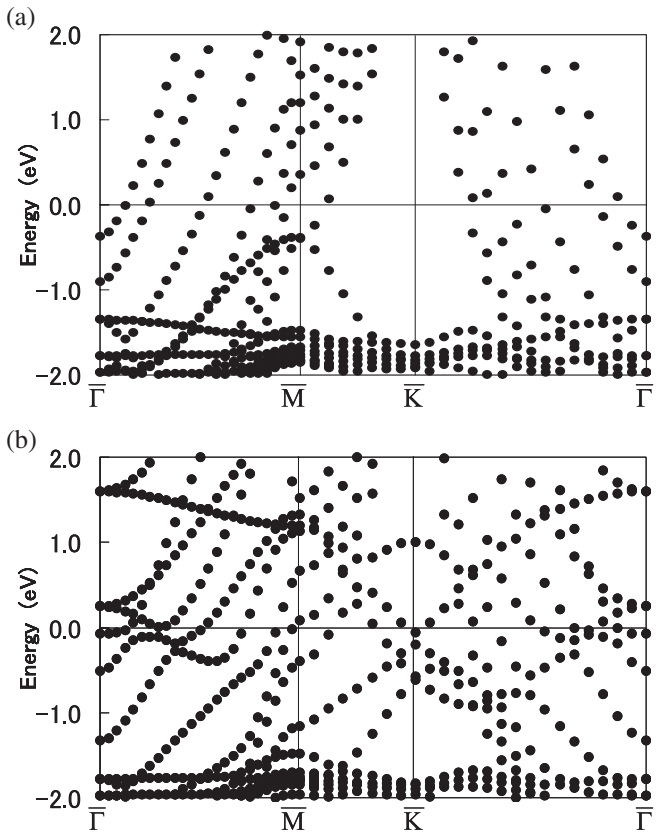

Figure 3. Band structures along the high symmetry direction for the majority spin electrons (a) and minority spin electrons (b). The Fermi level defines the energy scale reference.

4. Summary

We calculate the conductance through an Fe thin film on Cu(111) and find that the conductance decays with increasing tip distance. The conductance for minority spin electrons decays more rapidly than that for majority spin electrons. Such conductance decay is caused by the two-dimensional dispersion in the band structure. In our previous study of Fe nanowires on Cu(111) [7], there are some bands which have one-dimensional dispersion. Therefore, we think that the corresponding conductance through the nanowires on the Cu surface will propagate much farther than that considered here. These calculations for the Fe nanowires are now in progress.

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