Transport properties via surface localized states of Ru, Rh and Pd thin films on Ag(111)

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Abstract

We investigate the transport properties of some 4d transition metal (i.e. Ru, Rh and Pd) thin films fabricated on Ag(111) based on first principles calculation. We calculate the conductance observed by double tipped scanning tunnelling microscope and find that the conductances through Ru and Rh thin films are majority spin polarized. We discuss these results and compare them with our previous study for Fe thin films.

Keywords

nanospintronics, thin films, ruthenium, rhodium, palladium

1. Introduction

The properties of nanostructures, such as magnetic thin films, nanowires and quantum dots on nonmagnetic metal surfaces have been a matter of intensive research for decades [1-6]. This is due to their unique properties such as enhanced magnetic moments and their potential applications to spintronics devices. There is a fascinating and delicate interaction between the structure of the ultrathin films and the underlying substrate producing the unusual electronic and magnetic properties. Recently, the ferromagnetic Fe thin film on Cu(111) can be fabricated layer-by-layer with the laser molecular beam epitaxy technique, and their magnetic properties are investigated by surface magneto-optical Kerr effect (SMOKE) and x-ray magnetic circular dichroism (XMCD)[1]. We have investigated the Fe, Co, Ni thin films on Cu(111)[3-5], and found that the enhanced magnetic moment is due to the decrease in coordination number of the transition metals and the enlarged lattice constant. We have also studied the band structure of these systems and discussed the transport properties which are useful for designing and realizing spintronics materials and/or devices.

In order to design these new materials and devices, it is important to examine various elements with their magnetic and transport properties on solid surfaces. Here, we are interested in 4d transition metals, particularly Ru, Rh and Pd. Although these elements exhibit nonmagnetic properties in the bulk system, they become ferromagnetic at nanometer scale, e.g. thin films, nanowires and nanoparticles[7-13]. Some 4d transition metals monolayers exhibit ferromagnetic properties on solid surfaces because of two-dimensional band-structure effect as mentioned in the studies of Blügel[7, 9]. According to Redinger *et al.*, Ru and Rh monolayers on Ag(111) also exhibit ferromagnetic states with $1.23 \mu_B$ and $0.67 \mu_B$, respectively[10]. Though these studies discuss the magnetic properties of Ru and Rh, to our knowledge, there has been no report regarding the corresponding transport properties of these materials. Hence, in this paper, we investigate the transport properties of these 4d transition metal thin films and compare them with our previous study on Fe thin films. In the next

section, we briefly present the computational procedure. In section 3, we present the numerical results and discussions. In the last section, we summarize the investigation.

2. Computational details

The slab model for Ag(111) consists of five atomic layers, as shown in Fig. 1. We use the plane-wave and ultrasoft pseudopotential code to determine the electronic structure of these systems [16]. The nonlinear core correction is employed where the core radius r_0 is 1.0 bohr for each atoms. The plane-wave set is cut off at kinetic energies of 26 Ry for Ru, 28 Ry for Rh and 30 Ry for Pd. To sample the two-dimensional Brillouin zone, we use 18 k-points for optimizing the structure and 2353 k-points for obtaining the corresponding band structure. For the exchange correlation energy, we adopted the generalized gradient approximation (GGA). We also calculate the cases with ferromagnetic and antiferromagnetic state in the 2x2 unit cells [3]. By performing the total energy calculations, we found that ferromagnetic states are more stable than antiferromagnetic states. For the calculation of conductance, we adopt the model for a double-tipped scanning tunnelling microscope (STM)[14, 15]. 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. This yields

$$\sigma = \frac{2\pi e^2}{\hbar} \Gamma_1 \Gamma_2 \left| \sum_n \frac{\Psi_n(\mathbf{r}_1) \Psi_n^*(\mathbf{r}_2)}{\mathcal{E}_F - \mathcal{E}_n} \right|^2, \quad (1)$$

where $\Psi_n(\mathbf{r}_i)$ is the one-electron wave function at the position of tip i , and $\mathcal{E}_n$ is the energy eigenvalue. Γ_i is a function with a period of the surface unit cell which describes the tip-sample coupling. The eigenvalues and wavefunctions are obtained by first principles calculations as mentioned above.

3. Results and discussion

We show the energy band structures of our systems in Figs. 2, 3 and 4. The calculated magnetic moments are $1.40 \mu_B$ (Ru), $0.70 \mu_B$ (Rh) and $0.00 \mu_B$ (Pd) which are comparable with the value by Redinger *et al*[10]. However, in this study, the interlayer spacings between 4d transition atoms and Ag are optimized, $2.30 \text{ \AA}$ (Ru), $2.28 \text{ \AA}$ (Rh) and $2.28 \text{ \AA}$ (Pd). They are 1.7%(Ru) and 0.1%(Rh) longer than those of the earlier studies. Consequently, the hybridization between 4d transition atoms and Ag weakens and the magnetic moments are slightly larger. For Pd case, the interlayer spacing is 1% smaller, nevertheless the magnetic moment remain vanished. There are some bands whose wave function is localized around the thin films which are indicated by white circles in Figs 2-4. This localization is not as strong as the case of Fe thin films on Cu(111) as shown by the concentric circles in Fig. 5. Bigger circles are demonstrated on the Ru case, showing a less localized wave function. Some of these surface localized state bands exist in the projected band gap of Ag(111). These bands contribute to the transport properties, which are observable by using double tipped STM[14]. The calculated conductances along Γ –M direction are shown in Fig. 6. These conductances decay with oscillation as the distance between the tips increases, which is also observed in the case of Fe thin films on Cu(111)[5]. This is due to the two-dimensional dispersion of the band structure. The oscillations of the conductances consist of peaks for different periods. The arrow on Fig. 6 (a) indicates the wave number corresponding to the period of the conductance peak. This wave number agrees with the wave number where bands cross the Fermi level as indicated by arrow in Fig. 2(a). Thus, the peaks of the period of conductance oscillations reflect the Fermi wave numbers.

In the case of Ru on Ag(111), the conductance is majority spin polarized as shown in Fig. 6(a). This is because the surface localized state bands for minority spin electrons of Ru thin films on Ag (111) are energetically located far from the Fermi level. Whereas the bands for majority spin electrons lie around the Fermi level as shown in Fig. 2(b) and 2(a),

respectively. Figure 6(d) shows the conductance for Fe thin film on Cu(111). Here, the surface localized bands for minority spin electrons are closer to the Fermi level than that for majority spin electrons in Γ -M direction [4, 5]. The corresponding conductance is thus minority spin polarized in contrast to that for the Ru thin films. For Fe thin films, the amplitude of conductance oscillations is small and the difference in conductance is slight, because there are no surface localized state bands across the Fermi level. The magnetic moment of Ru ($1.4 \mu_B$) is smaller by $1.3 \mu_B$ but the spin polarization of conductance is larger than that of Fe. In the case of Rh thin films on Ag (111), since the surface localized state bands for majority spin electrons are as far from the Fermi level as those for the minority spin electrons (Fig. 3(a) and 3(b)), the spin polarization is smaller as compared to that of Ru thin films (Fig. 6(b)). Lastly, the conductance for Pd thin films does not have large peak (Fig. 6(c)) because the surface localized state bands lie relatively far from the Fermi level as shown in Fig. 4.

4. Summary

We have investigated the transport properties of 4d transition metals (Ru, Rh, Pd) thin films on Ag(111) observed by double tipped STM. Using the density functional theory-based calculations, we have calculated the conductance of the thin films on Ag(111) as a function of distance between tips. We find that the conductance decays with oscillation corresponding to the Fermi wave number as the distance between tips increases, and the conductances through Ru and Rh thin films are majority spin polarized. Moreover, we find that spin polarization of conductance of Ru is larger than that of Fe, while the magnetic moment is smaller. The spin polarization of the conductance depends on the position of the surface localized bands. These surface localized state bands of materials contribute greatly in designing surface spintronics devices.

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Figure Captions

Fig. 1. Schematic description of the model system.

Fig. 2. Band structures of Ru thin films on Ag(111) for (a)majority spin electrons and (b)minority spin electrons. The Fermi level, E_F , defines the energy scale reference. Surface localized states are indicated by white circles.

Fig. 3. Same as Fig. 3, but showing the case of Rh thin films.

Fig. 4. Same as Fig. 3, but showing the case of Pd thin films.

Fig. 5. Distribution of the one electron wave function for (a)Ru thin film on Ag(111) and (b) Fe thin film on Cu(111). Gray circles indicate Ru or Fe atom and white circles indicate Ag or Cu atoms.

Fig. 6. The conductance for (a)Ru, (b)Rh, (c)Pd and (d)Fe[5] thin films on Ag(111) along the Γ -M direction. For Ru and Rh, the conductances of majority and minority spin electrons for Ru, Rh and Pd are plotted by solid and dotted lines, respectively. The origin of the distance corresponds to the position of tip 1.

Fig. 1

Fig. 2

Fig. 3

Fig. 4

Fig. 5

Fig. 6(a)

Fig. 6(b)

Fig. 6(c)

Fig. 6(d)