Exchange interaction between magnetic adatoms on surfaces of noble metals

E. Simon,[1] B. Újfalussy,[2] B. Lazarovits,[2] A. Szilva,[3] L. Szunyogh,[3] and G. M. Stocks[4]

[1]*Lóránd Eötvös University, Department of Physics, HU-1518 Budapest POB 32, Hungary*

[2]*Research Institute for Solid State Physics and Optics of the Hungarian Academy of Sciences, Konkoly-Thege M. út 29-33., HU-1121 Budapest, Hungary*

[3]*Department of Theoretical Physics, Budapest University of Technology and Economics, Budafoki út 8., HU-1111 Budapest, Hungary*

[4]*Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA*

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We present first-principles calculations of the exchange interactions between magnetic impurities deposited on (001), (110), and (111) surfaces of Cu and Au and analyze them, in particular, in the asymptotic regime. For the (110) and the (111) surfaces, we demonstrate that the interaction shows an oscillatory behavior as a function of the distance, R, of the impurities and that the amplitude of the oscillations decays as $1/R^2$. Furthermore, the frequency of the oscillations is closely related to the length of the Fermi vector of the surface states existing on these surfaces. Due to the asymmetry of the surface-states dispersion, the frequency of the oscillations becomes also asymmetric on the (110) surfaces, while on the Au(111) surface two distinct frequencies are found in the oscillations as a consequence of the Bychkov-Rashba splitting of the surface states. Remarkably, no long-range oscillations of the exchange interaction are observed for the (001) surfaces where the surface states are unoccupied. When burying the impurities beneath the surface layer, oscillations mediated by the bulk states become visible.

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I. INTRODUCTION

The Rudermann-Kittel-Kasuya-Yoshida (RKKY) interaction in bulk materials is known for a long time,[1] and has become a textbook knowledge. In the past two decades, also the oscillatory exchange coupling in magnetic multilayers has been extensively studied both in experiment[2,3] and in theory.[4–6] Recently, surface nanostructures containing only a few, or even just one atom, were fabricated, and the exchange interaction between the individual atoms could be measured directly.[7,8] Various aspects of this interaction have already been discussed from first principles.[9–14]

In bulk, the magnitude of the RKKY interaction decays as $1/R^3$, where R is the distance between the impurities, and the extremal vectors of the Fermi surface determine the frequency of the oscillatory interaction. It is well known that the (111) surface of noble metals contains Shockley-type surface states[15–18] that behave as a two-dimensional free-electron gas (2DEG). It has been shown even earlier that the 2DEG mediates an RKKY type of interaction between magnetic impurities that has the asymptotic form $\sin(2k_F R)/R^2$, where k_F is the radius of the Fermi surface (circle).[19–24]

The study of realistic, more complicated (non-free-electron-like), Fermi surfaces or the absence of a (partially) occupied surface state call for more elaborate theoretical tools. Such methods account for the semi–infinite host system beneath the surface by calculating the surface Green function from first principles.[25,26] Previous studies of the exchange interaction at surfaces concentrated merely on the (001) and (111) surfaces of the host material being mostly copper,[9–14] and a comparative study of the vicinal surfaces of different host materials is still missing or incomplete, especially regarding the asymptotic regime.

In the present work, we perform calculations for the (100), (110), and (111) surfaces of Cu and Au in order to understand the role of various surface properties and their influence on the frequency and amplitude of the exchange interactions between Co atoms placed on these surfaces. It is well known that in the case of Au(111) the large spin–orbit interaction results in a splitting of the surface-states dispersion, called the Bychkov-Rashba splitting.[15,17,18,27,28] Here, we demonstrate how the Bychkov-Rashba splitting manifests itself in the exchange interaction on Au(111) and also on Au(110) surfaces.

II. METHOD OF CALCULATION

The screened-Korringa-Kohn-Rostoker (SKKR) method[29,30] combined with the embedding technique[26] enables a precise treatment of a finite cluster of impurities embedded into a two-dimensional translationally invariant semi-infinite host. Within multiple-scattering theory, the electronic structure of a cluster of embedded atoms, C, is described by the corresponding scattering-path-operator (SPO) matrix, $\tau_C(\epsilon)$ (ϵ being the energy), given by the following Dyson equation:[26]

$$\tau_C(\epsilon) = \tau_h(\epsilon)\left\{1 - \left[t_h^{-1}(\epsilon) - t_C^{-1}(\epsilon)\right]\tau_h(\epsilon)\right\}^{-1}, \qquad (1)$$

where $t_h(\epsilon)$ and $\tau_h(\epsilon)$ denote the single-site scattering matrix and the SPO matrix of the unperturbed host sites at the place of cluster C, respectively, while $t_C(\epsilon)$ stands for the single-site scattering matrix of the embedded atoms. Self-consistent calculations within the local-density approximation (LDA) of the density-functional theory (DFT) can then be easily performed.[30] In the present calculations no attempt was made to include surface relaxations: the cluster and the host sites refer to the positions of an ideal fcc lattice with the experimental lattice constant of Cu ($a_{\mathrm{fcc}} = 3.6147$ Å) and Au ($a_{\mathrm{fcc}} = 4.0648$ Å). Surface relaxations can largely influence the magnetic properties of adatoms,[31] thus, most likely also the magnitude of the exchange interaction between them. In the present study we, however, focus on the conditions under which long-ranged interactions between adatoms exist on a metallic surface, in particular, on the periods of asymptotic

oscillations that, as we shall show, are not affected by specific properties of the impurities.

First, we performed self-consistent (relativistic) calculations for the (001), (110), and the (111) surfaces of Cu and Au, then for Co impurities placed on the top of these surfaces. The details of the self-consistent calculations are described in Ref. 26. Once the self-consistent potential and exchange field for a single impurity has been obtained, we used the magnetic-force theorem[32] to calculate the interaction between two magnetic impurities. As in this procedure the relaxation of the electronic structure due to the proximity of the impurities is neglected, the exchange interaction between two impurities should be calculated from the grand canonical potential, $\Omega = E_{\rm band} - \epsilon_F N$, with $E_{\rm band}$, ϵ_F, and N being the band energy, the Fermi level, and the number of valence electrons, respectively.

For uniaxial systems, such as considered in this paper, the dependence of the grand potential on the orientations of the magnetic moments, $\vec{e}_1$ and $\vec{e}_2$, can be written up to second order as[33,34]

$$\Omega(\vec{e}_1,\vec{e}_2;\vec{R}) = \Omega_0(\vec{R}) + K\left(e_1^z\right)^2 + K\left(e_2^z\right)^2 + \tfrac{1}{2}\,\vec{e}_1\,\mathbf{J}(\vec{R})\,\vec{e}_2, \tag{2}$$

where K is the uniaxial-anisotropy constant of a single impurity and $\mathbf{J}(\vec{R})$ is a 3×3 matrix comprising the isotropic, symmetric anisotropic, and the asymmetric exchange (Dzyaloshinskii-Moriya) interactions between two impurities placed at a relative position, $\vec{R}$.

As usual, we define the exchange-coupling energy between two impurities as

$$J(\vec{e};\vec{R}) = \Omega(\vec{e},\vec{e};\vec{R}) - \Omega(\vec{e},-\vec{e};\vec{R}), \tag{3}$$

a quantity that still depends on the orientation, $\vec{e}$. From Eq. (2) we, however, see that the uniaxial-magnetic-anisotropy terms that can be of order of meV's drop from $J(\vec{e};\vec{R})$,

$$J(\vec{e};\vec{R}) = J(\vec{R}) + \vec{e}\,\mathbf{J}^{\rm sym}(\vec{R})\,\vec{e}, \tag{4}$$

where

$$J(\vec{R}) = {\rm Tr}\mathbf{J}(\vec{R})/3 \tag{5}$$

is the isotropic-exchange-coupling parameter and

$$\mathbf{J}^{\rm sym}(\vec{R}) = \tfrac{1}{2}(\mathbf{J}(\vec{R}) + \mathbf{J}(\vec{R})^T) - J(\vec{R})\mathbf{I} \tag{6}$$

is the traceless symmetric part of $\mathbf{J}(\vec{R})$ with the unit matrix $\mathbf{I}$. It should be noted that the so-called symmetric exchange (two-site anisotropy), $\mathbf{J}^{\rm sym}(\vec{R})$, arises purely from relativistic effects and it scales with the squared spin-orbit-coupling strength. Since our calculations indicate that this term is much smaller in magnitude than the isotropic exchange coupling, in this study we disregard the orientational dependence of $J(\vec{e};\vec{R})$ and present calculations of Eq. (3) at the specific orientation, $\vec{e} = \hat{z}$. In order to carefully trace the long-range oscillations of $J(\vec{R})$, when calculating the host τ_h matrices, see Eq. (1), we used 30 000 $k_{||}$ points in the irreducible wedge of the surface Brillouin zone, while 10 000 $k_{||}$ points were sufficient to use in the absence of occupied surface states.

In Table I, calculated exchange interactions are shown between adatoms at selected distances for the case of a Cu(111) surface. Note that negative/positive values indicate ferromagnetic/antiferromagnetic coupling between the spins. Two approaches are compared: (i) using single-impurity potentials as described above and (ii) taking into account the proximity of the two impurities in terms of self-consistent calculations. We denote the respective results for the exchange interactions by $J_{1i}(\vec{R})$ and $J_{2i}(\vec{R})$. As expected, for impurities at large distances ($R = 10\,a$ and $20\,a$, where a is the nearest-neighbor distance) the two methods are in reasonable agreement. For the nearest-neighbor pair, however, the exchange energy obtained from self-consistent two-impurity potentials are roughly twice as big as the ones calculated from the single-impurity approach.

TABLE I. Exchange interactions between Co impurities at selected distances, R (in units of the nearest-neighbor distance, a), on a Cu(111) surface as calculated by two different approaches (see text).

R/a	J_{1i}	J_{2i}
1	−197 meV	−106 meV
10	−24.5 μeV	−24.3 μeV
20	1.29 μeV	1.31 μeV

Finally, it should be pointed out that in the calculations presented in this work the relaxation of the electronic structure between the magnetic adatom and the host is neglected. This seems to be a crude approximation, however, as we checked for the case of Cu(110) surface, beyond a distance of about 20–30 Å no significant change in $J(R)$ is caused when including the first nearest-neighbor host shell with respect to the single-site approach. The reasoning of this observation is that the Cu (noble metal) atoms are very weakly polarized by the magnetic adatoms. Clearly, for the case of highly polarizable hosts, like Pt, Pd, or W, the single-site approach would considerably fail.[31,36]

III. RESULTS AND DISCUSSION

A. Nearest-neighbor interactions

Although the main purpose of the current paper is to investigate the asymptotic behavior of the magnetic interaction between two surface impurities, we would like to briefly comment on the nearest-neighbor interactions as well. For two impurities that are close enough to have sufficient overlap of their wave functions, it is the direct exchange that dominates the interaction. It gives a strong, but short-range coupling that decreases rapidly. We compare the exchange energy for nearest-neighbor impurities in bulk and on surface as calculated from the single-impurity approach (see above). As we have seen, for the nearest-neighbor pairs this is a crude approach, but it provides a qualitative estimate for the desired comparison. It is again worth to notice that taking into account surface relaxations, including also lateral distortions, is essential in exploring the electronic and magnetic structure of dimers (or small atomic clusters).[35]

Our results for Cu and Au hosts are presented in Table II. In both cases the coupling of the two Co spins is ferromagnetic in the bulk. This interaction is largely enhanced at the (100) and (111) surfaces. In general, this enhancement can be correlated with the decreased number of host atoms in nearest-neighbor

TABLE II. Calculated nearest-neighbor exchange interactions in bulk and on different surfaces of Cu and Au.

Host	Surface	J_{surf}(meV)	J_{bulk}(meV)
Cu	100	−198	−48.9
	110	10.5	
	111	−197	
Au	100	−109	−38.5
	110	7.85	
	111	−135	

positions below the Co atoms, four for (100) and three for (111), correspondingly, with a decreased hybridization between the Co and host atoms. Though very small in magnitude, on top of the (110) surface the nearest-neighbor exchange interactions become antiferromagnetic. This observation clearly demonstrates that the surface electronic structure can dramatically change the interactions between adatoms as compared to the bulk.

B. Asymptotic behavior

We calculated the exchange interactions, $J(R)$, between two Co adatoms deposited on top of the (111), (110), and (100) surfaces of Cu and Au for distances up to $R \simeq 100$–150 Å, to be considered safely as the asymptotic region. The calculated results are shown in Fig. 1 as a function of the distance between the adatoms. In case of the (100) and the (111) surfaces, the two Co atoms were placed along the (110) direction, i.e., the nearest-neighbor direction, while in case of the (110) surface along the (001) direction, i.e., the next-nearest- neighbor direction.

For the (111) surface of Cu, see left-top panel of Fig. 1, $J(R)$ shows clear oscillations with a period of $L = 18.5$ Å, corresponding to a Fermi wavelength of the surface states, $k_F = \pi/L = 0.17$ 1/Å. This period is very close to the value $L = 15$ Å, or $k_F = 0.22$ 1/Å, obtained from STM measurements and also from first-principles calculations by Stepanyuk *et al.*[11,12] The difference between the theoretical results can mostly be attributed to the different angular momentum cutoffs and surface potentials used in the calculations. In agreement with theoretical models,[19–24] our numerical fit also confirmed that the amplitude of the oscillations decays as $1/R^2$.

The asymptotic curve of $J(R)$ displays a more complicated behavior for Au(111), see right-top panel of Fig. 1, since this curve could be fitted as the sum of two oscillations with the Fermi wavelengths $k_F^1 = 0.104$ 1/Å and $k_F^2 = 0.142$ 1/Å. The appearance of the two oscillation periods is due to the famous Bychkov-Rashba splitting[27] of the Au(111) surface states experiencing the strong spin-orbit interaction of Au. This splitting of the surface states gives rise to two distinct spherical Fermi cuts, thus, to two distinct asymptotic oscillations for the exchange interaction between magnetic adatoms. It should be noted, however, that, mainly because of the imprecise treatment of the surface potential within the ASA, our values for the Fermi wavelengths are typically smaller, while their difference, $\Delta k_F = 0.038$ 1/Å, is larger than reported in the literature.[15–17]

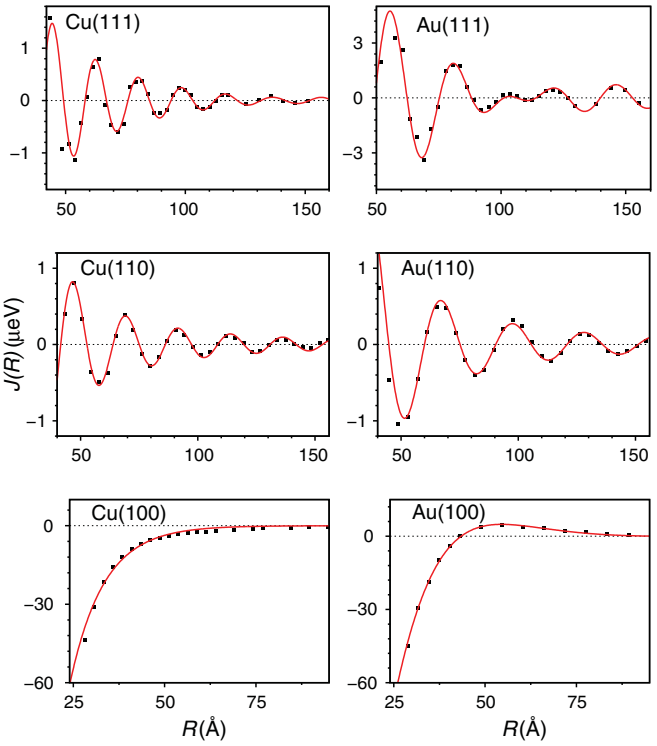

FIG. 1. (Color online) Calculated exchange interactions as a function of the distance between Co adatoms on top of the vicinal surfaces of Cu and Au along the directions specified in the text. Symbols refer to the calculated data, solid lines to the fitted curves.

As studied by Petersen *et al.* in terms of Fourier-transformed scanning-tunneling microscopy (STM),[37] there exist partially occupied Shockley states on the Cu(110) surface that are located at the boundary ($\overline{Y}$ point) of the two-dimensional Brillouin zone. These surface states naturally give rise to oscillatory exchange interactions between magnetic adatoms as demonstrated in the middle panels of Fig. 1, both for Cu(110) and Au(110) surfaces.

Noticeably, the shape of the cuts of these surface states is elliptic due to the C_{2v} symmetry of the surface. Consequently, the period of the oscillations depends on the direction along which the two adatoms are pulled apart.[38] Figure 2 presents the exchange interactions in the case of Cu(110) along the (001) and the $(1\bar{1}0)$ directions. The Fermi wavelengths obtained from fitting these curves, 0.141 1/Å and 0.172 1/Å along the (001) and the $(1\bar{1}0)$ directions, agree indeed very well with the values derived directly from the dispersion relation of the surface states, 0.138 1/Å and 0.164 1/Å, respectively.

In the case of Au(110), we observed two oscillations in $J(R)$ along the (001) direction, corresponding to the Fermi wavelengths 0.098 1/Å and 0.118 1/Å. Similar to Au(111), this can again be explained by the fact that the Au(110) surface states experience an anisotropic Bychkov-Rashba splitting.[39] Note, however, that the amplitude of the oscillation with the longer period ($k_F = 0.098$ 1/Å) turned out to be about 16 times larger than the one for the shorter period ($k_F = 0.118$ 1/Å). Most likely, an even larger imbalance of the amplitudes applies to the asymptotic exchange interactions along the direction $(1\bar{1}0)$, since in this case it was not possible to resolve

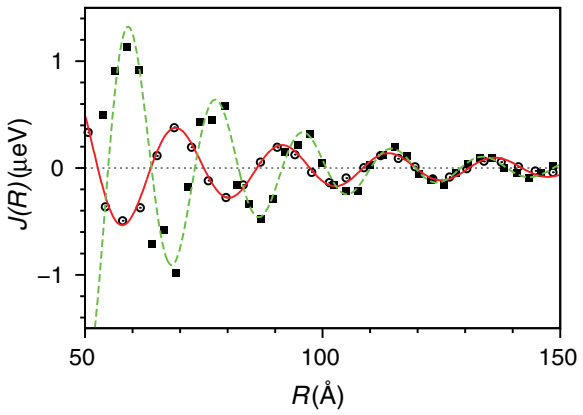

FIG. 2. (Color online) Calculated exchange interaction on the Cu(110) surface along two different directions: (001) (circle) and $(1\bar{1}0)$ (filled square). The solid and dashed lines correspond to the fitted curves.

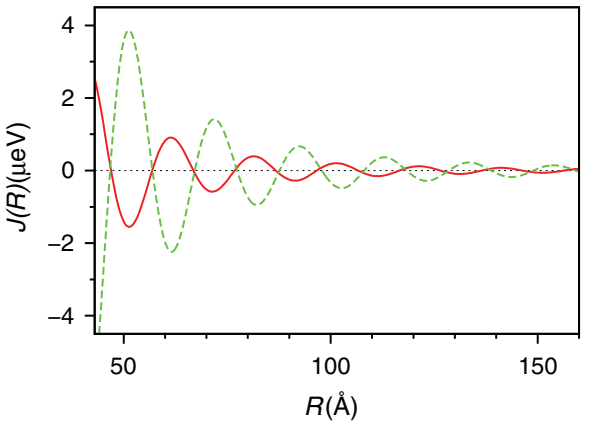

FIG. 4. (Color online) Fitting curve of the calculated exchange interactions between two Fe (dashed line) and Co (solid line) adatoms placed on top of a Cu(110) surface along the $(1\bar{1}\bar{1})$ direction.

numerically the two different frequencies in the oscillations, our fit confirmed only the short period with $k_F = 0.151$ 1/Å.

In obvious contrast to all previous cases, in the case of the (100) surfaces (lower panels of Fig. 1) the exchange interactions show no oscillations in the asymptotic regime. For Cu(100), $J(R)$ is well described by an exponential decay. For Au(100), it also rapidly decreases with R, though, $J(R)$ changes sign at $R \simeq 30$ Å. Therefore, we may conclude that, lacking (occupied) free-electron-type surface states, there is no long-range RKKY-type exchange interaction between the magnetic atoms on the (100) surfaces. At first glance, this statement contradicts the observation of Stepanyuk *et al.*,[10] who established an oscillatory coupling even in the case of Cu(100). Their calculations were, however, restricted to distances $R < 10$ Å, which can not be regarded as the asymptotic regime.

However, once the Co adatoms are placed in the surface layer, an oscillatory exchange interaction appears, although with a different frequency than in the bulk, see right-top panel of Fig. 3 for the case of Cu(100) surface. When placing the impurities even deeper beneath the surface, the frequency of the bulk RKKY interaction is quickly recovered. It is well known that the Cu Fermi surface has four extremal vectors along the (110) direction.[5] Among them, the largest one, related to the (110) diameter of the "dog-bone"–shaped Fermi surface, causes the rapid oscillations in the bulk as seen on the bottom-right panel of Fig. 3. Interestingly, our numerical analysis shows that the frequency of the oscillations for adatoms in the surface (S) layer correlates with the much shorter extremal vector of the Fermi "neck".

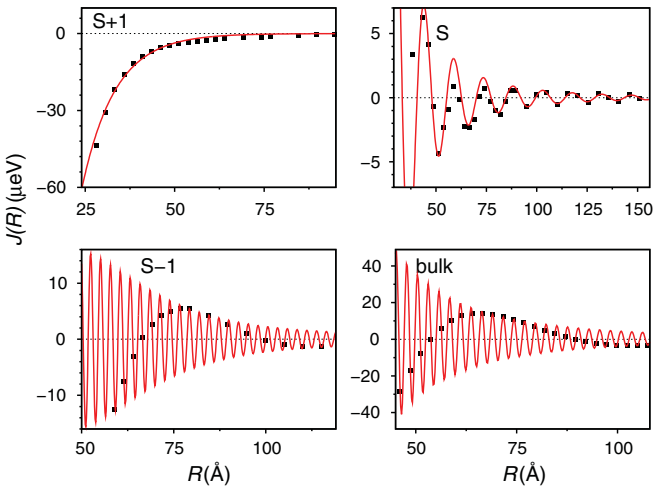

FIG. 3. (Color online) Calculated exchange interactions between two Co impurities placed at different vertical positions with respect to a Cu(100) surface: $S + 1$ on top, S in the surface layer, and $S - 1$ in the subsurface layer, as well as in the bulk.

So far, we presented numerical results for the exchange interaction between two Co impurities. In Fig. 4 the exchange interactions between two Co adatoms are compared with that between two Fe adatoms placed on top of Cu(110) surface along the $(1\bar{1}\bar{1})$ direction. From this figure, it can clearly be inferred that the frequency of the asymptotic oscillations is the same for both cases: the type of the adatoms is manifested in the amplitude and in the phase of the oscillations. The period of $L = 20.4$ Å corresponds to a Fermi wavelength of $k_F = 0.154$ 1/Å, which, reassuringly, coincides well with the length of the spanning vector of the elliptical Fermi-surface cut along the corresponding direction.

IV. CONCLUSION

We presented first-principles calculations of the exchange interactions between magnetic impurities deposited on the vicinal surfaces of Cu and Au. In full agreement with previous theoretical studies, for the (110) and the (111) surfaces we demonstrated that the interaction in the asymptotic regime is oscillatory: the amplitude decays as $1/R^2$, where R is the distance of the adatoms, and the frequency of the oscillations coincides with the length of the Fermi vector of the Shockley-type surface states existing on these surfaces. In the case of the (110) surfaces, the surface states around the $\bar{Y}$ point of the surface Brillouin zone have an elliptic paraboloid dispersion relation, due to the C_{2v} point-group symmetry. This, in turn, resulted in an anisotropic periodicity of the exchange interaction when varying the direction between the adatoms. Moreover, for the Au(111) surface two distinct

frequencies are found in the oscillations at any direction as a consequence of the Bychkov-Rashba splitting of the surface states.

Our most remarkable observation is the lack of long-range oscillations in the asymptotic exchange interaction for the (001) surfaces. This finding can be correlated with the fact that there are no partially occupied surface states in this case. We should note that the bulk Fermi-surface-related oscillations decaying as $1/R^5$ predicted by Lau and Kohn[21] could not be numerically resolved in our calculated data. When burying, however, the impurities beneath the surface layer, oscillations mediated by the bulk states become apparent.

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