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Anisotropy of exchange interactions between impurities on Cu(110) surface

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Abstract. We study the exchange interaction between two magnetic impurities on the (110) surface of Cu. We find that the interaction is oscillatory and decays as $1/d^2$ for large distances d of the impurities. We also show that the oscillations are governed by the Shockley-type surface state around the $\overline{\mathrm{Y}}$ point of the Surface Brillouin zone. The asymmetry of the dispersion of this surface electronic band implies an anisotropic exchange interaction with respect to the relative position of the impurities.

1. Introduction

The L-gap Shockley-type surface states on the (111) surface of noble metals, that form a quasi two-dimensional electron gas, have been investigated rather extensively, both experimentally [1] and theoretically [2, 3]. This surface states are of particular importance, because they give rise to enhanced interactions between impurities placed on the (111) surface which can also lead to the formation of self-organized nanostructures [4, 5]. In case of the Au(111) surface, a characteristic splitting of the surface state due to the large spin-orbit coupling has been observed by photoemission and photoelectron spectroscopy [6, 7]. A theoretical interpretation of this splitting was given by Henk *et al.* [8] in terms of a Rashba-type Hamiltonian and ab initio calculations.

In this work we investigate the consequence of the surface states related to the Cu(110) surface that arise from a relative gap at the Fermi level around the $\overline{\mathrm{Y}}$ point of the Surface Brillouin zone (see Figure 1.). In terms of ab initio calculations we show that these surface states also induce interactions between magnetic impurities. Unlike the case of the (111) surface, the periodicity of the asymptotic oscillations depends on the relative orientation of the impurities.

2. Computational details

First we performed self-consistent, relativistic calculations for a single Co impurity on the Cu(110) surface by using the embedded-cluster technique within the multiple scattering theory (MST) [9]. This method enables a formally exact treatment of a finite cluster of impurities embedded into a two-dimensional translational invariant semi-infinite host. Within MST the

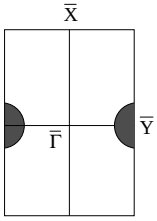

Figure 1. Brillouin zone of the fcc(110) surface. The shaded area marks the projection of the relative gap of the Fermi Surface.

electronic structure of a cluster of embedded atoms is described by the so-called scattering path operator (SPO) matrix given by the following Dyson equation [9],

$$\tau_C(\epsilon) = \tau_h(\epsilon)[1 - (t_h^{-1}(\epsilon) - t_C^{-1}(\epsilon))\tau_h(\epsilon)]^{-1} \quad , \tag{1}$$

where $\tau_C(\epsilon)$ comprises the SPO for all sites of a given finite cluster C embedded in a host system, $t_h(\epsilon)$ and $\tau_h(\epsilon)$ denote the single-site scattering matrix and the SPO of the unperturbed host sites in cluster C, respectively, while $t_C(\epsilon)$ stands for the single-site scattering matrix of the impurity atoms. Self-consistency is achieved using the local density functional of Ceperley-Alder (in the parameterization due to Perdew and Zunger) [10] and solving the Poisson equation as described in Ref. [9]. In the self-consistent calculation for the embedded atom the orientation of the magnetization was chosen to point uniformly along the surface normal (z axis) and the atomic sphere approximation (ASA) was applied. The host and the cluster sites referred to the positions of an ideal *fcc* lattice with the experimental lattice constant of Cu ($a = 3.6147$ Å), neglecting thus structural relaxations of the impurity and the host atoms near the surface.

The interaction between two impurities deposited on the surface has been calculated by using the magnetic force theorem [11], i.e., neglecting further self-consistency effects. This implies that only the band- (single particle) energy has to be considered. The exchange interaction between impurities placed at sites $\vec{R}_1$ and $\vec{R}_2$ is defined by

$$\Delta E = E(\uparrow \vec{R}_1, \uparrow \vec{R}_2) - E(\uparrow \vec{R}_1, \downarrow \vec{R}_2)\,, \tag{2}$$

where arrows stand for the magnetic orientations of the impurities: $\uparrow$ for z and $\downarrow$ for $-z$.

3. Results

It is widely known that in metallic bulk systems and for large distances $d = |\vec{R}_1 - \vec{R}_2|$ the Rudermann-Kittel-Kasuya-Yoshida (RKKY) interaction between magnetic impurities decays as $\cos(2\pi d/\lambda)/d^3$ where the period of the oscillations, λ, is related to the length of an extremal vector of the Fermi surface, $2k_F$, namely, $\lambda = \pi/k_F$. For impurities at surfaces with a Shockley-state as mentioned in the Introduction, a similar RKKY interaction pertains, though, with a decay of $1/d^2$ [12]. The most studied case refers to the magnetic impurities on the surface of Cu(111) induced by the L-gap related surface state. At the Fermi energy this surface state appears as a circle of radius k_F centered at the $\overline{\Gamma}$ point of the SBZ and results in an isotropic interaction $\sim \cos(2k_F d)/d^2$ as shown in terms of ab initio calculations by Stepanyuk et al. [4].

In the case of the (110) surface, however, the projection of the Fermi surface results in a gap that is at the boundary of the two dimensional Brillouin zone, see Figure 1. It can also be seen that the shape of this gap is non-spherical. By performing ab-initio calculations as described above, in very good agreement with experiments [13], we found that there exists an occupied surface state. By calculating the dispersion relation of this surface state we found

this to be asymmetric around the $\overline{\mathrm{Y}}$ point as it is shown of Figure 2. The cross section of the surface state dispersion at the Fermi energy $E(k_x, k_y) = E_F$ is no longer circular, similar to the projection of the gap, it is distorted as well. This distortion is than results in a different $2k_F$ in various directions: $2k_F^x$=0.148 1/Bohr and $2k_F^y$=0.174 1/Bohr. Note that in our notation x and y corresponds to the directions (001) and $(1\bar{1}0)$, respectively.

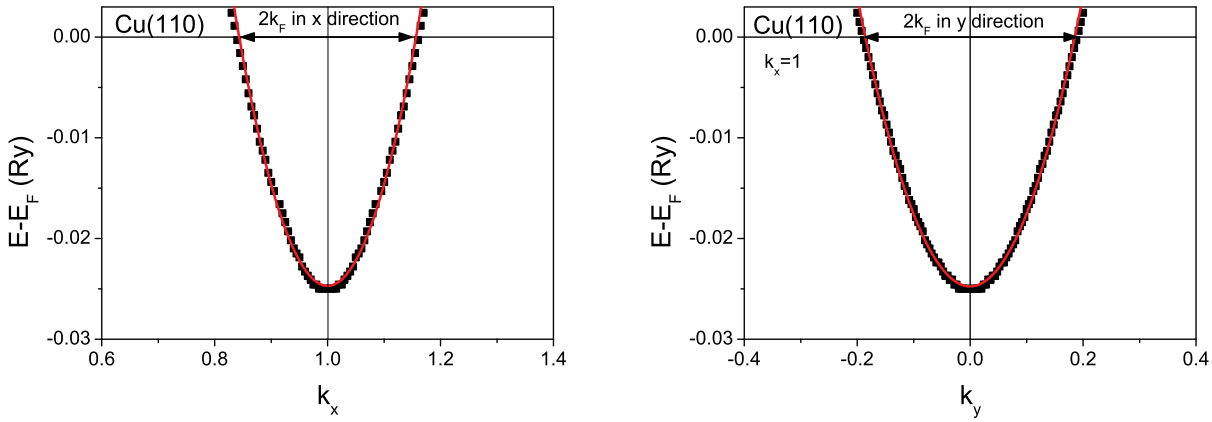

Figure 2. Calculated dispersion relations of the surface state around the $\overline{\mathrm{Y}}$ point of the Cu(110) Brillouin zone. Left panel: $k_y = 0$, right panel: $k_x = \pi/a$ (a is the 2D lattice constant).

The question than naturally arises whether this asymmetry will result in an anisotropic impurity-impurity interaction on the (110) surface. The results of our calculations of Eq. (2) can be seen in Figure 3. We found that it is indeed the case: the period of the oscillations of ΔE depends on the direction along which the two surface impurities are placed. In the asymptotic regime, ΔE as a function of d can also be fitted as mentioned above. From this fit the obtained frequencies of oscillations, 0.160 1/Bohr for the x direction and 0.183 1/Bohr for the y direction, are in good agreement with the calculated $2k_F$ values of the surface state's dispersions.

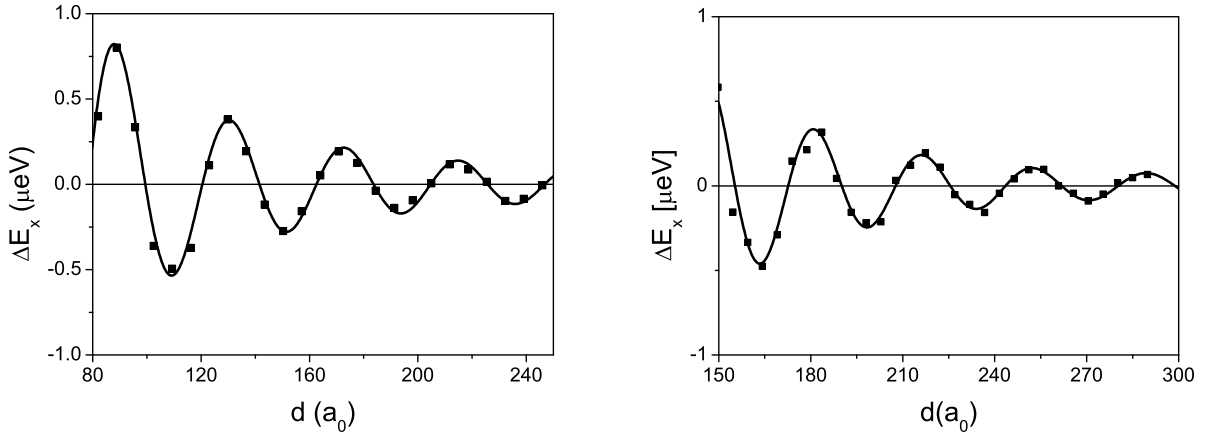

Figure 3. Calculated exchange interaction energies (squares) and fitted curves (solid lines) on Cu(110). On the left: the distance of the impurities, d, is varied along the (001) direction, on the right: along the $(1\bar{1}0)$ direction.

4. Conclusions

We performed ab initio calculations for the surface states and surface Co impurities on Cu(110). We found that the surface state dispersion is asymmetric around the $\overline{\mathrm{Y}}$ point of the 2D Brillouin zone. This asymmetry manifests itself in an anisotropy of the impurity-impurity exchange interaction. These results further establishes the role of Shockley-type surface states as mediators of the interaction between impurities at surfaces. Further studies are planned to explore the observed phenomenon in context of the Ag(110) and Au(110) surfaces, in particular, its possible implications on the Rashba splitting of the corresponding surface states.

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