Supporting Online Material for

Seeing the Fermi Surface in Real Space by Nanoscale Electron Focusing

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1 Supporting Online Material

Materials and Methods 1: Experiment Setup

The preparation was carried out using a UHV metal-epitaxy chamber directly attachable to a home-built low temperature STM which was used for the measurements. The subsurface impurities have been prepared by simultaneous deposition of host metal and the impurity material on clean single crystal surfaces using two electron beam evaporators. One of them, operating at moderate fluencies ($\approx 1$ layer/min), performs a homoepitactical growth of the matrix material. The second one, kept at very low deposition rates, carries out an admixture of the impurity atoms at specific times during the growth process by pulsed shutter operation. A more detailed description of the STM and the preparation chamber can be found in (1).

Materials and Methods 2: Ab intio Method

In the present work we use the full–potential KKR Green function method (2) within the local spin density approximation. This method is ideal for treating systems involving impurities on or in surfaces and in bulk crystals. Within the KKR method the impurities are described by considering a cluster of perturbed atomic potentials which includes the potentials of the impurities and the perturbed potentials of several neighbor shells. Also in the vacuum region the space is filled by cellular potentials, of which the ones close to the impurity are perturbed (as compared to the clean surface). The impurity potential and the perturbed potentials of the neighboring cells are embedded in an otherwise ideal unperturbed surface.

The KKR method is based on multiple–scattering theory. For non–overlapping potentials the following angular momentum representation of the Green function $G(r + R_n, r' + R_{n'}; E)$ can be derived:

$$G(r + R_n, r' + R_{n'}; E) = -i\sqrt{E} \sum_L R^n_L(r < ; E) H^n_L(r >; E) \delta_{nn'} + \sum_{LL'} R^n_L(r; E) G^{nn'}_{LL'}(E) R'^n_{L'}(r'; E).$$

Here $E$ is the energy and $R_n, R_{n'}$ refer to the atomic positions. $r_<$ and $r_>$ denote respectively the shorter and longer of the vectors $r$ and $r'$ which define the position in the Wigner–Seitz (WS) cell centered around $R_n$ or $R_{n'}$. The $R^n_L(r; E)$ and $H^n_L(r; E)$ are respectively the regular and irregular solution of the Schrödinger equation.

The structural Green functions $G^{nn'}_{LL'}(E)$ are then obtained by solving the Dyson equation for each spin direction

$$G^{nn'}_{LL'}(E) = \tilde{G}_{LL'}^{nn'}(E) + \sum_{n'',L''L'''} \tilde{G}_{LL'''}^{nn''}(E) \Delta t^{n''}_{L''L'''}(E) \tilde{G}_{L'''}^{nn''}_{LL'}(E).$$

(1)

The summation in (1) is over all lattice sites $n''$ and angular momenta $L''$, $L'''$ for which the perturbation $\Delta t^{n''}_{L''L'''}(E) = t^{n''}_{L''L'''}(E) - \tilde{t}^{n''}_{L''L'''}(E)$ between the $t$ matrices of the real and the reference system is significant. $\tilde{G}_{LL'}^{nn'}$ are the structural Green function of the reference system, i.e. in our case the ideal Cu(111), Cu(001) or Cu/Co(111) surfaces.
According to the Tersoff-Hamann model (3) the scanning tunnelling spectra can be related to the s-DOS induced by the surface or by the adatom at the position of the STM tip. Adopting this model, we calculate the s-LDOS at a distance $z = 6.1 \, \AA$ directly above the center of the surface layer.

**Supporting Text: Spin-filter Idea**

We simulated an interface of Cu/Co(111) using a slab of Cu (Fig. 5A) in which we replaced 6 layers of copper by cobalt. Below the Cu surface (and above the interface) we placed a Co impurity which leads to the vacuum CDO shown in Fig. 5B. The striking effect is the appearance of two additional rings. The outer ring has in fact been already observed with the pure Cu slab i.e. it is the result of the scattering of the electrons waves at the second surface of the slab. The inner ring however is due to the scattering at the Co interface. This has been verified using the trigonometrical relations mentioned in the main text. The black circles plotted in Fig. 5B are the demonstration that our explanation is very plausible. We tried to exploit the idea of spin-filtering by looking at the spin-resolved charge variation assuming a ferromagnetic coupling between the Co impurity and the Co interface. In the left of Fig. 5C, the majority-spin is depicted while in the right the minority-spin is shown. We have focused on the intensities of the outer region from the first triangle that we hidden by an orange disk. The main result here is that the second ring of the majority-spin has lower intensities compared to the second ring of the minority-spin. This is explained by the fact that Co majority FS is very similar to the FS of Cu (it has a filled majority band) whereas the minority-spin FS is different. In addition, one notices a phase shift between the minority and majority oscillations: when there is a positive intensity (in red) in the right picture of Fig. 5C we see a negative intensity (in blue or blue green) in the left picture.

**References**


Figure S1: (A) Slabs used in the ab-initio simulations showing that the waves going directly to the vacuum-side lead to a first inner ring while the ones reflected at the Cu/Co interface reflection lead to an additional ring. (B) Charge variation due to the presence of a Co impurity at 12.14 Å below a Cu(111) surface. Size of the vacuum charge shown is 10 nm by 10 nm. The outer ring is created after reflection of the waves at the other side of the slab. (C) Spin-resolved charge variation in the same system. The first triangle is hidden by an orange disk in order to focus on the intensities of the second and third rings. The majority-spin charge is characterized by lower intensities for the middle ring compared to the minority-spin charge since the majority electrons are practically not scattered at the Cu/Co interface. The Co-interface plays here the role of spin-filter (see text for more details).