The electron wave function at a vicinal surface: mixed terrace/average-surface behavior in Cu(10 10 13)

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Vicinal surfaces can be used as model systems to study the basic features of the electronic structure in a lateral superlattice. In particular noble metal (111) surfaces which are characterized by the presence of a free-electron-like surface band that can be easily probed in angle-resolved-photoemission. One of the fundamental questions concerns the electron wave function that propagates in the direction perpendicular to the lattice. Does the electron follow the average surface corrugation or is it rather attached to the terrace planes. The two possibilities are schematically displayed on top of Fig. 1. Although terrace and average-surface modulation are expected respectively for low and high step densities, it is not obvious what is the critical miscut angle for a switch-over. As shown in Fig. 1, the critical miscut angle from terrace to average-surface wave function modulation at vicinal Cu(111) lies between 5º and 9º. This result has been proved recently at HASYLAB by means of angle-resolved, photon-energy-dependent photoemission and using a diffraction-like scheme for data analysis [1]. The latter is shown in the bottom panels in Fig. 1. The data points (dots) represent the final-state photoelectron wave vector inside the Cu crystal for electrons at the bottom of the surface state band. Both parallel and perpendicular components are determined from the photoemission data assuming the usual energy and parallel wave vector conservation within the constant-inner potential approximation. There is a qualitative change in the data obtained for different miscut angles. For large (9º) miscut (small terraces, left) data points lie at a fixed parallel momentum at the edge of the surface Brillouin zone. For small (5º) miscut (large terraces, right), they line along the [111] direction. To understand this difference it is necessary to have a close view to the surface state wave function, in particular to its evanescent part along the perpendicular direction (Fig 1, top). Due to the strong confinement within the surface, the wave function has a broad distribution of perpendicular wave vectors, which are separately picked up by varying photon energy. As it is shown in Fig. 1 by means of the shaded cigars, in Cu such a distribution is centered around the center of the gap, i.e. the *L* point in the bulk band structure. For 9º miscut, we obtain the expected result for a regular surface state on the average terrace plane [2]. For 5º miscut, however, the results are consistent with a wave vector spread in the direction perpendicular to the (111) terraces, thus

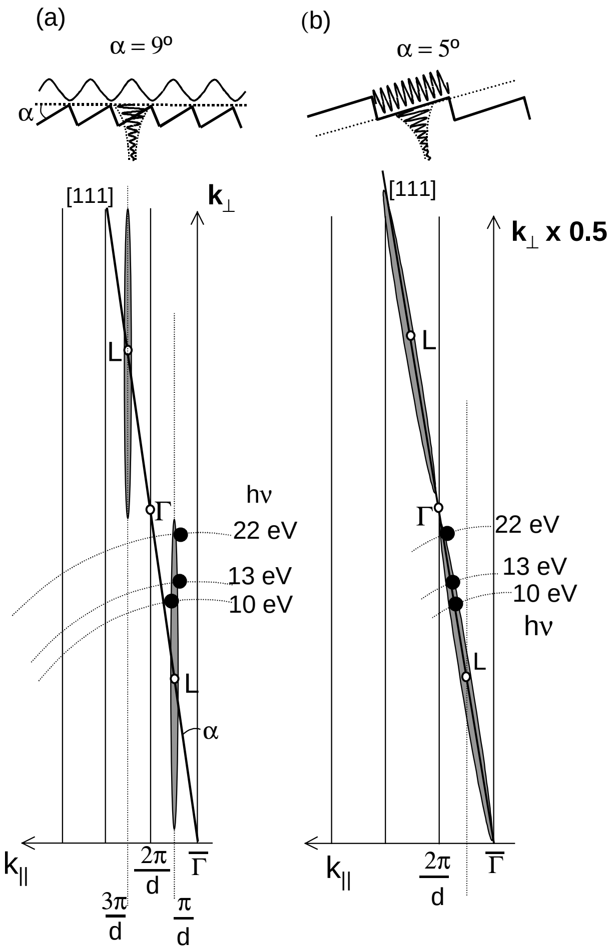

Fig. 1. Bottom, description of the photoemission experiment from a vicinal surface using an electron diffraction model. The dots are three-dimensional k-values obtained from the data in Fig. 2 via Eqs. 1 and 3. The cigar-shaped, hatched regions represent the spread of the surface state wave function in k- space. The corresponding wave function in real space is indicated on top. A characteristic switch of the orientation occurs at a critical miscut angle between 5º and 9º.

indicating that the wave function is modulated along this direction.

In order to further confirm these observations, we have performed new experiments on a 7° miscut vicinal Cu(111) (namely, Cu(10 10 13)) during our 1999 beamtime at the F2.2 beamline in HASYLAB (Winkelemi setup). The results are shown on Fig. 2, left. The photoemission intensity (dark) is plotted as a function of the energy relative to E_F and the emission angle with respect to the average surface. The parabolic fit helps to locate the band minimum in each case. From the position of this band minimum we have calculated the perpendicular and parallel components of the final state wave vector (Fig. 2 right, red dots) . The data points display the expected behavior for a transition from a terrace-modulated wave function (see Fig. 1, 5° miscut) to an average-surface modulated one (9° miscut in Fig. 1). Thereby for 7° miscut surfaces (17 Å wide terraces in average) the surface state wave function appears to be basically described by two different Fourier components, i.e. one shaping the step lattice corrugation and the other one reflecting the atomic corrugation of the (111) terraces.

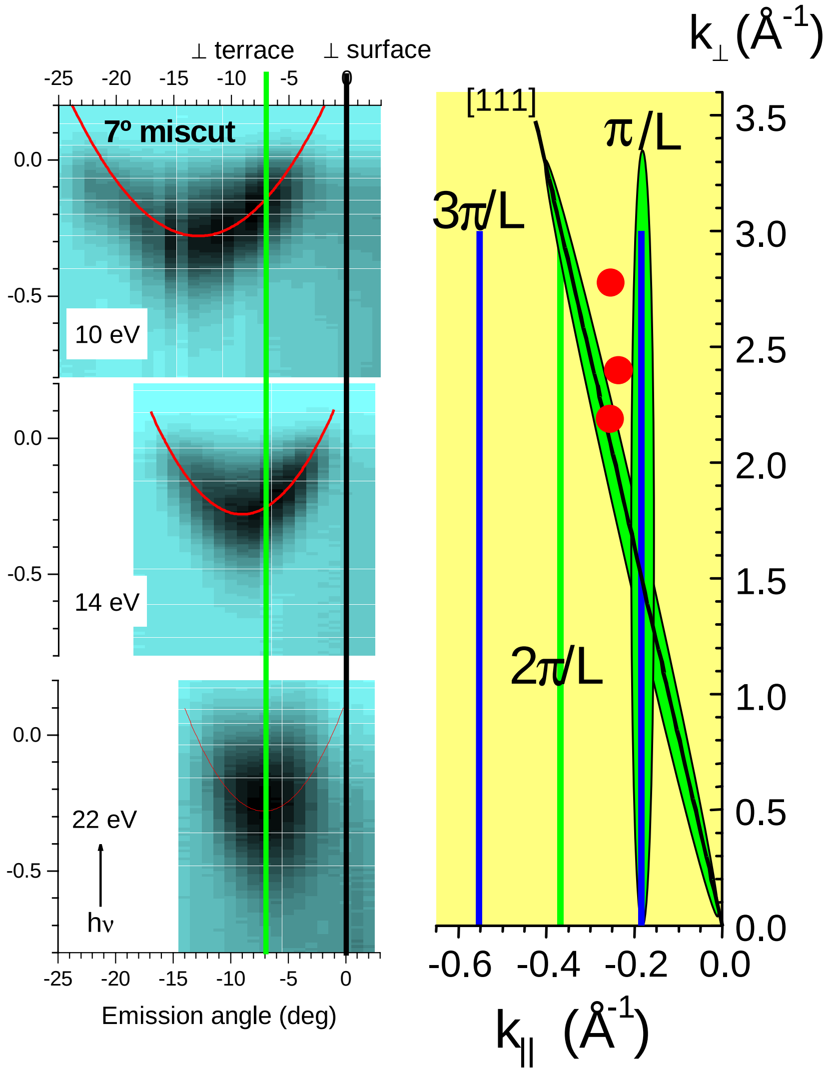

Fig. 2. Left, Photoemission intensity versus energy and emission angle taken with different photon energies showing the p_z-like surface state in Cu(10 10 13). The two wave vector components (right, red dots) are calculated for the band minimum. The location of the data points between the surface normal at L and the (111) direction (cigars) indicate a mixed terrace-average-surface wave function modulation.

This work has been supported by the EC through the TMR program (Project N° ERBFMGECTP950059). Additional funding from the Universidad del País Vasco (UPV057.240-EA026/98) and the Spanish Ministry of Education (DGES, PB-970031) is acknowledged.

References

1. "The electron wave function at a vicinal surface: Switch from terrace to step modulation", J. E. Ortega, S. Speller, A. Bachmann, A. Mascaraque, E. G. Michel, A. Mugarza, A. Närmann, A. Rubio, and F. Himpsel, Phys. Rev. Lett. (submitted).
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