ELECTRONIC PROPERTIES OF KINKED AND BRANCHED MONATOMIC QUANTUM WIRES

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A low-temperature scanning tunneling microscope (LT-STM) operating at 7 K is used to build kinked and branched Cu chains on a Cu(111) surface by means of lateral manipulation of single adatoms. It has been shown that straight monatomic Cu/Cu(111) chains exhibit localized electronic states (Fig. 1) trapped in the pseudo gap of the projected Cu bulk bands [1] and thereby constitute a clear-cut model system for a 1D quantum wire. The energies of these states are well described by the linear combination of atomic orbitals (LCAO) approach with the two parameters α=3.31 eV and β=-0.96 eV corresponding to the coulomb integral and the resonance integral, respectively. The good agreement is attributed to the fact that the single Cu/Cu(111) adatom is associated with a quasi-atomic resonance as revealed by density functional calculations [2] and experimentally verified by local spectroscopy. The quantum states are interpreted to derive from the coupling of these atomic resonances along the chain.

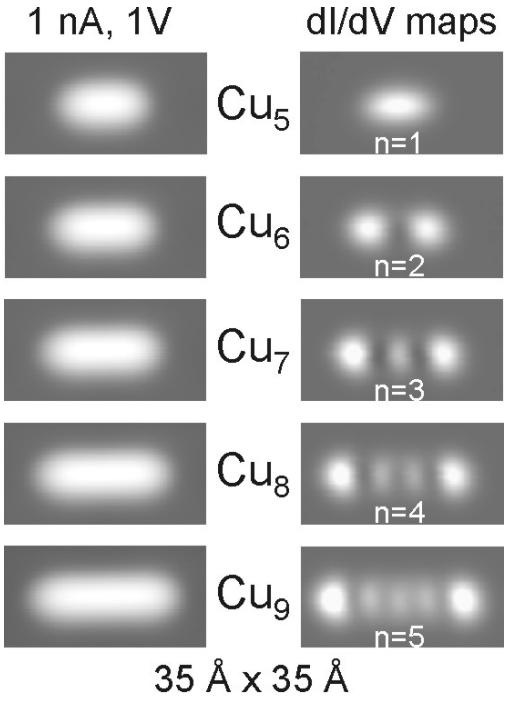

Fig. 1 *Constant-current STM images of monatomic Cu/Cu(111) chains consisting of five to nine atoms (left), and selected dI/dV maps (right); the indicated quantum number n specifies the number of wavefunction lobes. The dI/dV maps were measured at 1.7 V, 2.2 V, 2.7 V, 3.1 V, and 3.4 V sample bias, respectively (with increasing order n).*

We assembled kinked V-shaped Cu/Cu(111) chains which are stabilized by a compact Cu trimer at the junction of the two linear branches running along the close-packed Cu row directions of the substrate. These 60°-kinked wires exhibit specific quantum states: Measurements of the differential tunneling conductance dI/dV for different sizes of structures show that the eigenstate energies of kinked wires are different from those of straight wires containing the same number of atoms. We also find that the number of peaks appearing in the dI/dV spectra for symmetric structures (i.e. structures comprised of a compact trimer and linear branches of equal length) is lower than expected. To gain insight into this characteristic

behavior we compared the measurement with the energies obtained by a LCAO calculation which shows that the electronic parameters of the trimer atoms have to be modified to get a semi-quantitative agreement between measured and calculated energies. This is attributed to the different local environment of the three trimer atoms as compared to Cu atoms within straight monatomic chains.

Maps of the dI/dV signal recorded at fixed sample bias indicate how the local density of states (LDOS) of the chain-localized states is spatially distributed. While the fundamental state is characterized by the absence of nodes, the excited states appear to be more complex. In the case of symmetric kinks, some of the measured dI/dV maps reflect the superposition of two states which are not resolved experimentally. This mixing is due to the broadening of electronic levels characterized by a half width of about 0.6 eV. The states that can not be separated in the experiment are analyzed by calculating the square of the respective eigenstate wavefunction within the LCAO approach. The results show how the dI/dV map can be separated into two electronic states.

More recently we studied branched Y-shaped wires that exhibit quantum states with a fundamental level at around 1.2 eV which is clearly lower than in the case of the Cu kinks (~1.35 eV). The comparison with LCAO still suggests a modification of the electronic parameters accounting for the three atoms of the junction.

The combination of atomic manipulation and local spectroscopy as applied here allows in detail to study the electronic implications of junctions of monatomic quantum wires. A simple description based on the LCAO method is capable to provide insight into general electronic features of these structures of advanced complexity.

References:

[1] S. Fölsch et al., Phys. Rev. Lett. **92**, (2004) 56803
[2] F. E. Olsson et al., Phys. Rev. Lett. **93**, (2004) 206803