FINAL STATE EFFECTS IN PHOTOEMISSION OF ONE-DIMENSIONAL METALS

P. Starowicz[1,2], O. Gallus[1], Th. Pillo[1], Y. Baer[1]

[1]Institut de Physique, Université de Neuchâtel, rue A.-L. Breguet 1, 2000 Neuchâtel, Switzerland

[2]Institute of Physics, Jagellonian University, Reymonta 4, 30-059 Kraków, Poland

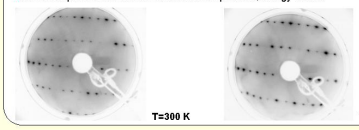
INVESTIGATED SYSTEM

PREPARATION

- Substrate: Si wafer, p-type, B-doped, with (335) surface cleaned by flashes at 1250 °C
- 0.28 monolayer of Au deposited and annealed at 800 °C forms a stable system of monoatomic steps and terraces (3x1 surface reconstruction)
- A monolayer of Na deposited on the "3x1 template" and partially desorbed by heating at 350 °C forms one dimensional structures - chains

LEED

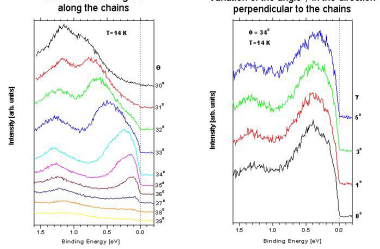
- 3x1 LEED patterns stable as a function of temperature, energy 125 eV



ANGLE RESOLVED PHOTOEMISSION RESULTS

Variation of the angle θ along the chains

Variation of the angle γ in the direction perpendicular to the chains

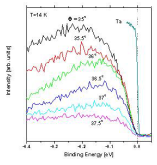


The observed peak approaches the Fermi energy. By extrapolation, it can be found that it would cross the Fermi level at 36°.

The peak vanishes gradually for further k values.

Neither Fermi step nor backfolding are visible.

The lack of dispersion in the direction perpendicular to the chains confirms 1-dimensional character of the band.



Qualitatively similar behaviour is observed in other photoemission studies of quasi one-dimensional systems, for example:

Bechgaard salts - F. Zwick et al., Phys. Rev. Lett. **79** (1997) 3982,

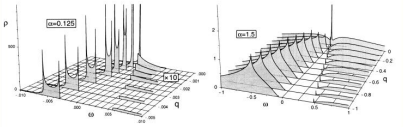
TTF-TCNQ - F. Zwick et al., Phys. Rev. Lett. **81** (1998) 2974, R. Claessen et al. Phys. Rev. Lett. **88** (2002) 6402,

$K_{0.3}MoO_3$, $Li_{0.9}Mo_6O_{17}$ - G. H. Gweon et al., J. Electron Spectrosc. Relat. Phenom. **117** (2001) 481

THIS BEHAVIOUR IS NOT UNDERSTOOD IN ANY FRAMEWORK OF EXISTING THEORIES

Spectral functions of a Luttinger liquid, ω=E-E$_F$ and q=k-k$_F$

J. Voit, J. Electron Spectrosc. Relat. Phenom., **117-118** (2001) 469



The observed data are not in agreement with the predictions of the **LUTTINGER LIQUID**, the linear behaviour close to E$_F$ would correspond to an unrealistic value of α=2 in the momentum-resolved spectral function: $A(\omega,k_F) \sim |\omega|^{\alpha-1}$

For a CONVENTIONAL METAL **(FERMI LIQUID)** a sharp metallic edge would be present while the band crosses the Fermi level. This would be well visible with our high energy resolution instrument (5 meV).

The absence of backfolding excludes an interpretation in terms of conventional band of SEMI-METAL or INSULATOR.

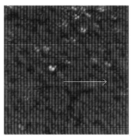
PROPOSED EXPLANATION

THE MODEL CONSIDERING SIZE EFFECTS AND COULOMB SHIFTS ALLOWS TO SIMULATE THE SPECTRA OFTEN OBSERVED IN PHOTOEMISSION OF 1-D SYSTEMS

PROPOSED SCENARIO

The impurities or lattice defects in one-dimensional systems may act as boundaries dividing these systems into small segments.

This role of the defects is unique to 1-D systems and the resulting segments of chains can be treated as clusters.

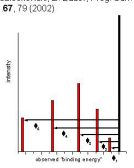


STM, Au chains on SI(533) surface

M. Jalochowski, E. Bauer, Prog. Surf. Sci **67**, 79 (2002)

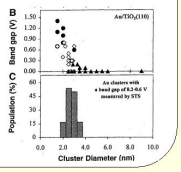
The photoemission process will leave these segments with a positive charge and the appropriate Coulomb shift will be added to the work function.

Each photo-excited level will contribute to the spectrum with different shifts depending on the chain lengths.



STM results for Au clusters on TiO$_2$:

M. Valden et al., Science **281** (1998) 1647.



INTRODUCTION OF THE MODEL

In photoemission, the observed energy ω will be shifted due to a Coulomb contribution to $\varepsilon = \omega + \phi(L)$

L - is the length of a chain segment or other size parameter for clusters

The suggested form of the ϕ function can be: $\phi(L) \propto \frac{\exp(-L/\lambda)}{L^m}$

where λ is adjustable attenuation length and $0 \le m \le 3$

In our current simulations: $m = 1$

The distribution of the chain lengths is assumed to be gaussian $G(L)$ with $\bar{L}$ - mean value and σ - full width at half maximum

$G(L)$ can be transformed into a shift distribution: $P(\phi)$

$$G(L)dL = G[L(\phi)]\frac{dL}{d\phi}d\phi = P(\phi)d\phi$$

If $A(\omega,k)$ is the spectral function for an infinite chain, the spectrum for the chain distribution is given by:

$$I(\varepsilon,k) = \int_{\omega<\varepsilon} A(\omega,k)P(\varepsilon-\omega)d\omega$$

Simulation of angle resolved spectra for 1-D systems

For k$_F$ we assume that the spectral function is a delta function at E$_F$:

$$A(\omega,k_F) = \delta(\omega)$$

Curves (**A**) and (**C**) are the simulations.

The parameters of curve (**A**) are:

$\sigma = 0.47\bar{L}$ $\lambda = 0.2\bar{L}$

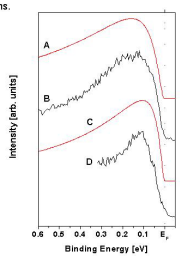
For the curve (**C**), σ and $\bar{L}$ have been increased by approximately 5% while the absolute value of λ remains the same as in simulation (**A**).

The spectra (**B**) and (**D**) are angle resolved photoemission measurements at k$_F$:

(**B**) is a spectrum for ϑ=36° for the currently discussed system

(**D**) is a result for SI(557)-Au reproduced from

P. Segovia, D. Purdie, M. Hengsberger and Y. Baer, Nature **402** (1999) 504



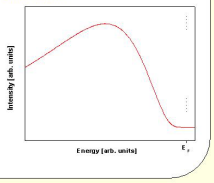
With increasing the size of chains (or clusters) the simulated spectrum approaches the Fermi level

Possibility of creating a pseudo-gap with the Coulomb Shift Model

used parameters:

$\sigma = 0.28\bar{L}$

$\lambda = 0.22\bar{L}$



Simulation of angle integrated spectra of a Fermi liquid in clusters

We assume constant $A(\omega)$ below E$_F$:

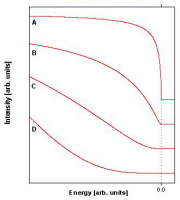
$$A(\omega) = \theta(\omega)$$

For the curve **A**: $\sigma = 0.59\bar{L}$ $\lambda = 0.13\bar{L}$

For the curves **B-D** λ remains constant, while the cluster size decreases:

SIMULATIONS

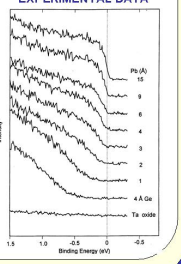
	$\bar{L}$	σ
A:		
B:	67% $\bar{L}$	67% σ
C:	50% $\bar{L}$	50% σ
D:	40% $\bar{L}$	37% σ



EXPERIMENTAL DATA

Angle integrated photoemission spectra from granular films of Pb evaporated on Ta oxide covered with two monolayers of Ge

D. J. Huang et al. Phys. Rev. B 55 R1977 (1997)



Reference: P. Starowicz, O. Gallus, Th. Pillo, and Y Baer, Phys. Rev. Lett. 89, 256402 (2002)

CONCLUSIONS

- The assumption that real one-dimensional systems are divided into segments which remain electrically charged after the process of photoemission provides an explanation of many experimental facts not understood in the framework of modern theories.
- This scenario sets strong limitations for the photoemission studies of 1-dimensional systems. However, samples with less defects or providing better screening will markedly improve the situation.