A STUDY OF THE PEIERLS – TRANSITION ON THE SYSTEM Br/Pt(110) BY SCANNING TUNNELING MICROSCOPY AND LOW ENERGY ELECTRON DIFFRACTION

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CHAPTER 6
SUMMARY AND OUTLOOK

This thesis aimed a further detailed characterisation of the system Br/Pt(110).The main experimental technique used was Scanning Tunneling Microscopy. In addition, Low Energy Electron diffraction and Thermodesorption mass spectrometry were used for controlling and preparing the different phases.
The main results are summarized below:

• Is there a possibility to prepare a global CDW – phase only by increasing the Br_2 – coverage without heating ? Is the annealing and the resulting dissociation of the Br atom pairs into individual atoms essential for the formation of the global phase ?

At additional Br_2 – coverages of ~ 0,02ML, a global (3×1) CDW phase is found even without annealing. For additional coverages up to ~ 0,003ML individual antiphase domains are present. The critical coverage, where the solitons spontaneously anneal (probably by CDW induced hopping of Br dimers) is very likely temperature dependent and needs further investigation. An explanation for the formation of a global phase only by increasing the coverage may be given in terms of the soliton energy. Accordingly, a reordering of the adsorbate atom pairs may take place, if the total soliton energy exceeds a critical value at higher coverages; then a global, commensurate structure is formed instead of the domains.
Annealing the global phase with Θ_{Br} (excess) = 0,02ML (~ 100°C) leads to the chain – like arrangement of Br – atoms along the $[1\,\bar{1}\,0]$ direction.The doping atoms are preferentially found in maxima but sometimes also in minima of the CDW, which is in accordance with previous results.

What is the nature of the CDW antiphase domains? Are they due to a commensurate CDW with randomly pinned phase (strong impurity pinning) or is there an incommensurate CDW at low coverages, which decays into commensurate antiphase domains (strong commensurability pinning)?

The NO doping experiments demonstrate that solitons resulting from the decomposition of an incommensurate CDW run preferably parallel to the (001) direction. Solitons at low Br coverages, in contrast, have no recognizable orientational preference (see, for instance, Fig. 5.11). Furthermore, a global (3×1) CDW is observed within a wide Br coverage range ($0{,}52 < \Theta_{Br} < 0{,}7$ ML. This indicates that the commensurability is only slowly changing with coverage. Hence, we conclude that the transition from CDW domains between 0,003ML and 0,02ML is caused by the increasing total soliton energy. At 0,02 ML it is large enough to render the antiphase domain structure unstable. Hopping of impurities brings them in phase and triggers the transition into the global CDW phase.

• What is the range of loss of atomic resolution of the c(2×2) – lattice and the decay lenghts of the (3×1) – domains at low coverages ?

By analyzing several images it was found, that the c(2×2) – lattice is distorted (resp. atomic resolution is lost) over large areas (> 100Å). It persists only were it is pinned at defects (steps etc.) or impurities.

In contrast, typical diameters of the (3×1) domains along the $[1\,\bar{1}\,0]$ and the [001] direction are 20 - 60Å. The largest diameters, however, are also of the order of 100 Å. Hence, even at the lowest coverages the domain size seems to be limited by the presence of neighbouring antiphase domains rather than a finite decay length.

Difficulties arise from the fact, that it is very hard to find areas without defects or impurities, which interact with the CDW's and therefore limit the domain size.

•Is it possible to prepare well - ordered phases with coverage well beyond Θ = 0,5ML when starting from a well – defined c(2×2) Br – overlayer ?

It is indeed possible to prepare a rather well - ordered (4×1) and a less well - ordered (8×1) – structure.

A detailed study of the (8×1) structure reveals local (3×1) structure elements, which arrange themselves in the observed (8×1) periodicity. The appearance of (3×1) structure elements separated by periodic phase discommensurations resembles the structures observed with NO doping. They may be attributable to an incommensurate CDW decomposing into locally commensurate (3×1) structures and solitons. Analysis of the coverage via TPD – spectra yields an additional coverage of 0,31ML compared with the c(2×2) – overlayer.

Similar considerations apply for the (4×1) – structure. TPD – spectra indicate an additional coverage of 0,1ML compared with the (8×1) – structure (i.e. Θ_{Br} (excess) ~ 0,4ML).

•Is it possible to prepare CDW's also by using alternative doping species ?

It was found, that CDW's do not spread around randomly distributed hole – defects, which were prepared by sputtering the surface. LEED shows only (1×1) – patterns.

In contrast, doping experiments using NO were successful: Two phases were identified in STM. At low coverages, a global commensurate (3×1) structure occurs. Increasing the coverage leads to the decomposition into local (3×1) domains, which alternate with NO zig – zag chains and solitons. Upon further NO exposure, the (3×1) structure elements and the zig – zag chains form a periodically alternating structure with 7 - fold periodicity. At a coverage of 0,25ML, a transformation into a commensurate (4×1) – phase, which is characterized by the zig – zag structures, takes place.

In observed NO phases, the NO is found to be very mobile on the surface. NO desorbs at temperatures slightly beyond room temperature; therefore the NO – substrate interaction is weak.

Experiments under progress indicate that CO behaves very similar to NO on the c(2×2) – Br/Pt(110) surface. It will be interesting to study other adsorbates and surface reactions after coadsorption on this peculiar surface.