



Experiment title: SXRD Study on the Structural Phase Transition of Pb/Si(557)

Experiment number:
Si 1759

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Report:

In the SXRD experiment, we wanted to elucidate the **structural origin** of the transition from **1D to 2D conductivity** for Pb monolayers on Si(557) by means of **SXRD** as it is essential for clarifying a new type of 1D conductance mechanism and its reversible transition. LEED studies suggest that the transition of conductivity from 1D to 2D is **forced by a phase transition of the surface structure** due to formation of **nano facets**. Therefore, this transition shall be investigated by means of SXRD to correlate temperature dependent transport (mesoscopic scale) with structural changes on the atomic scale.

Previous results:

a) Successful preparation and characterization of Si(557): Clean Si(557) samples have been prepared in the UHV chamber hosted at ID03 although the preparation is quite delicate. They have been characterized by means of SXRD. Refaceting due to too high flashing temperatures as well as sample holder induced stress to the samples have not been found. As obvious from in-plane scans presented in Fig.1, a (3x1) reconstruction along the H-direction (7, 7,-10) is seen in addition with GIXRD due to local step bunching forming (111) and (112) facets thus former experiments by Robinson et.al. [1] have been successfully reproduced. In some cases even a (6x1) reconstruction has been seen as the Si atoms are in-phase every six (557) units on this unequally stepped surface laterally. The high resolution GIXRD experiments could easily resolve these large unit cells (7.64nm) and contain therefore valuable information with respect to the macroscopically performed transport measurements, because STM can measure reliably only the local step structure. On the contrary, with LEED

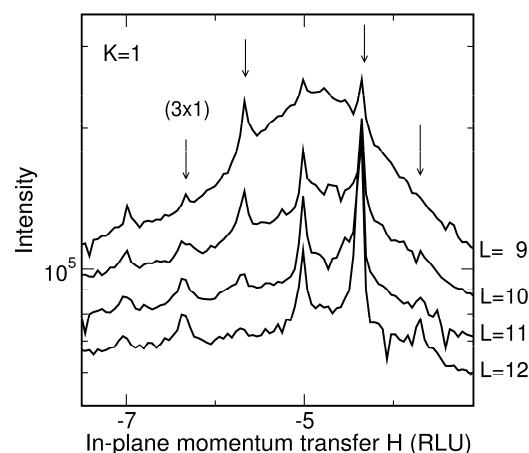


Figure 1: SXRD scans in the K=1 plane of clean Si(557) surface for different L-values. The Bragg peak is at (-5,1,7).

On the contrary, with LEED

the (3x1) reconstruction has not been seen due to the finite terrace size distribution and less resolution of the instrument [2].

b) Pb induced refacetting and formation of Pb nanowires: The evaporation of Pb was carried out around 180K substrate temperature. The evaporator could accurately be calibrated using XRR monitoring during deposition. GIXRD shows the formation of a single crystalline Pb film. Comparison of XRR and GIXRD reveals that the first 4 ML grow amorphously whereas crystalline growth was found for monolayers in addition. While adsorption at low temperatures does not change the former (557) orientation, new facets have been found after annealing. By monitoring a Pb-Bragg peak (lattice mismatch is 10% between Pb and Si) controlled desorption of multilayers was possible until the wetting layer remains on the vicinal surface, showing a $\sqrt{3}\times\sqrt{3}$ reconstruction. As obvious from Fig.2 the H-scans show the formation of the quasi-(223) (=17,17,25) facets where the separation of the reciprocal rods along H is increased by 21%. We emphasize particularly this preparation, as it demonstrates a homogeneously heating of the sample. In addition a splitting of 10% around the $\sqrt{3}$ position ($K=1.3$) at slightly different H allows provisionally the conclusion, that Pb nanowires on the (111) nanofacets have successfully been grown. From LEED experiments it is known that this corresponds to 1.3ML, i.e. the coverage which shows the intriguing phase transition in transport [3,4].

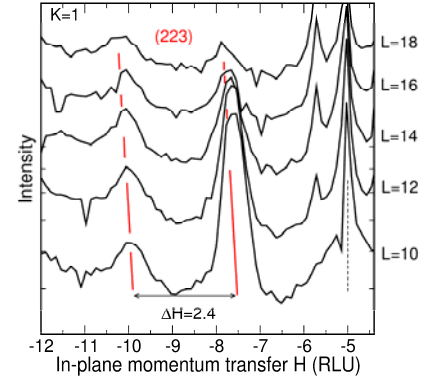


Figure 2: Formation of (223) facets after multilayer desorption. The remaining coverage of 1.3ML after desorption was deduced from the domain wall splitting.

c) First CTR measurements: For rods at different H-positions in the $K=1$ and $K=-1$ plane first fundamental CTRs have been measured. A first inspection shows an intensity modulation, i.e. information about Pb adsorption sites projected onto the $K=0$ plane might be obtained. The data analysis (with the *anarod* software) will improve significantly the model of the reconstruction on the nanofacets shown schematically in Fig.3 as deduced from LEED and STM.

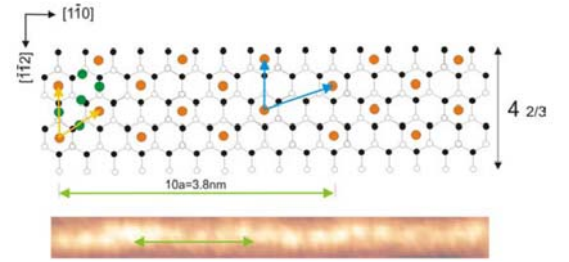


Figure 3: Model of the (1,5) phase of 1.31ML Pb on Si(557). The full monolayer structure is shown only for the first $\sqrt{3}$ cell.

Open questions:

- As temperatures below 180 K were not accessible during the beamline time, only measurements above T_c have been performed for the quasi-(223) facet structure. It turns out that the experimental setup is extremely stable with respect to changes in temperature (even after flashing a recalibration of the sample was not necessary), thus we expect that the phase transition can be measured during the cooling process. Fundamental CTRs need still to be measured at different temperatures.
- It was found that the ordering of the quasi-(223) facet structure can be improved by longer annealing times. It will be interesting to see, how the phase transition depends on the perfectness of the (223) facet structure. This is of importance, because previous transport measurements have been performed on a macroscopic sample [3].
- Finally, the $\sqrt{3}$ must be investigated in more detail. As LEED studies by us have shown only the domain splitting, SXRD has revealed already a substructure, which was not seen before. Furthermore, CTRs on $\sqrt{3}$ -reflex positions should be measured in order to allow an more accurate determination of the Pb atoms in the (H,K)-plane.

- [1] I.K. Robinson et.al. PRB 88 (2002) 096104.
- [2] M.Czubanowski et.al. NJP 9 (2007) 338.
- [2] C. Tegenkamp, et.al. PRL 95 (2005) 176804.
- [3] C. Tegenkamp, et.al. PRL 100 (2008) 076802.