


**Experiment title:**

Surface Phase Transition in Pb/Cu(100)

**Experiment number:**

25-02/649

|                           |   |                                    |
|---------------------------|---|------------------------------------|
| <b>Beamline:</b><br>BM25B | <b>Date of experiment:</b><br>from: 20/01/09 to: 26/01/09 | <b>Date of report:</b><br>26/02/09 |
| <b>Shifts:</b><br>21      | <b>Local contact(s):</b><br>Dr. German Rafael CASTRO      | <i>Received at ESRF:</i>           |

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**Report:**

Group metals III and IV absorbed on (100) oriented noble metals exhibit a rich variety of surface structures. The goal of this experiment was to characterized the phase transition dynamic between the phases  $c(5\sqrt{2}\times\sqrt{2})R45^\circ$  and  $(\sqrt{2}\times\sqrt{2})R45^\circ$  split, that take place in Pb/Cu(100) at 0.6ML and at 450 K (see **table I**). Our aim was also to study the cristallography of the phases involved in this transition, which would let us relate the electronic changes to the structural ones. The role of the electronic structure on this reversible phase transition is not clear yet, so this study could give light to its understanding. For the  $(\sqrt{2}\times\sqrt{2})R45^\circ$  split we proposed the same atomic structure as for the  $(5\times 5)R\ tg^{-1}(3/4)$  phase, which comprises square domains of  $(\sqrt{2}\times\sqrt{2})R45^\circ$  separated by wall domains.

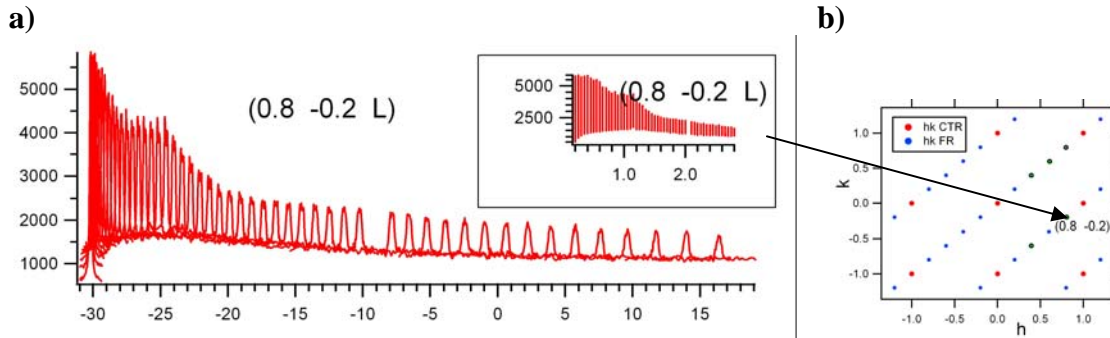
|    |   |  |   |   |  |
|----|---|--|---|---|--|
| HT |   |  |   |   | $(\sqrt{2}\times\sqrt{2})R45^\circ$ split<br>$\uparrow$ "c(2x2)" split<br>$T=450\ K$ |
| RT |   | $(2\sqrt{2}\times 2\sqrt{2})R45^\circ$<br>" c(4x4) " | $\sqrt{2}\times\sqrt{2}R45^\circ$<br>" c(2x2) " | $\sqrt{2}\times\sqrt{2}R45^\circ$ split <b>II</b> c<br>" c(2x2) " split | $c(5\sqrt{2}\times\sqrt{2})R45^\circ$<br>$\downarrow$                                |
| LT | $\sqrt{61}\times\sqrt{61}\ R\ \tan^{-1}(5/6)$ |  | $(3\sqrt{2}\times\sqrt{2})R45^\circ$            | $\approx(5\times 5)R\ tg^{-1}(3/4)$                                     |  |
| ML | 0.24  | 3/8  | 1/2   | 0.5-0.6   | 6/10   |

**Table I** Phase diagram of Pb/Cu(100) in the monolayer regime (horizontal axis) as a function of temperature (vertical axis)

**Results:**

We obtained a good sample quality both in the clean and Pb-evaporated samples. The technical problems we had in the previous beamtime with the sample annealing are completely solved. We have succesfully

prepared the phase  $c(5\sqrt{2} \times \sqrt{2})R45^\circ$  and characterized it by measuring three CTR's, five fractional rods and in-planes along five directions. In **fig.1** we show a fractional rod at  $(0.8 -0.2 L)$ , with  $l=0.2-2.8$ .

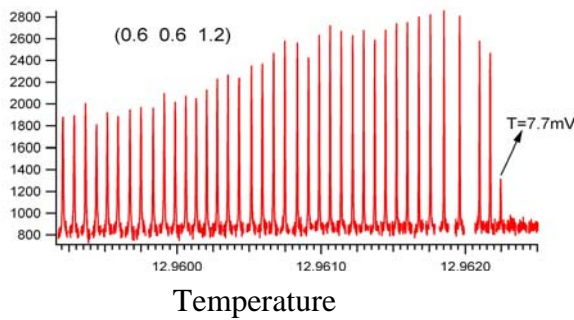


**Fig.1a)** Superposition of fractional rod spectra vs phi at  $(0.8 -0.2)$  for different  $l$  values. In the inset we plotted the same vs  $l$ ;

**b)**  $(hk)$  diagram of the phase  $c(5\sqrt{2} \times \sqrt{2})R45^\circ$ ; the measured fractional rods are highlighted in green.

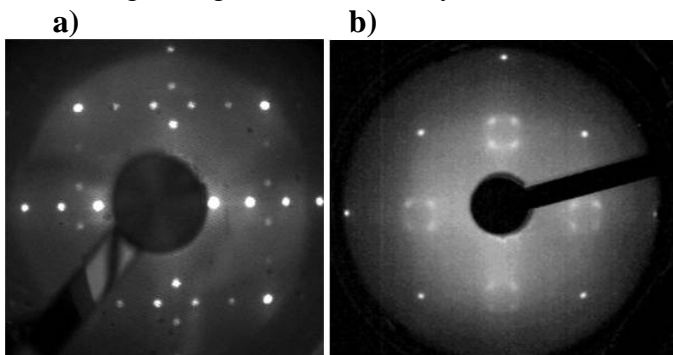
The quality of the peaks reveals the formation of a good surface and the possibility of analyzing the surface crystallography of this phase.

Once characterized this phase, we started annealing the sample to reach the  $(\sqrt{2} \times \sqrt{2})R45^\circ$  split phase. In **fig.2** we followed the spot  $(0.6 0.6 1.2)$  from the  $c(5\sqrt{2} \times \sqrt{2})R45^\circ$  phase during the sample annealing until it disappeared.



**Fig.2** Intensity of the  $(0.6 0.6 1.2)$  spot from the  $c(5\sqrt{2} \times \sqrt{2})R45^\circ$  phase vs the sample temperature.

We could not find the spots of the  $(\sqrt{2} \times \sqrt{2})R45^\circ$  split phase by SXRD. Even though this phase should have shown a LEED pattern as pictured in **Fig.3b**, we could not check it due to technical problems. A closer inspection to previous LEED patterns of the  $(\sqrt{2} \times \sqrt{2})R45^\circ$  split phase, as the one in **Fig.3b**, reveals that its background is prominent. We should evaluate the possibility that the domains of the  $(\sqrt{2} \times \sqrt{2})R45^\circ$  split phase are not big enough to be studied by SXRD.



**Fig.3 a)** LEED pattern of the  $c(5\sqrt{2} \times \sqrt{2})R45^\circ$  phase and **b)** of the  $(\sqrt{2} \times \sqrt{2})R45^\circ$  split phase.

## Conclusion:

The good performance of the diffractometer and the rest of the beamline let us got a complete data set to characterize the atomic structure of the  $c(5\sqrt{2} \times \sqrt{2})R45^\circ$  phase. Further SXRD and complementary studies (STM) are needed to characterized the  $(\sqrt{2} \times \sqrt{2})R45^\circ$  split phase.