



	<b>Experiment title:</b> Structural analysis of a surface charge density wave phase transition in In/Cu(100)	<b>Experiment number:</b> SI-930
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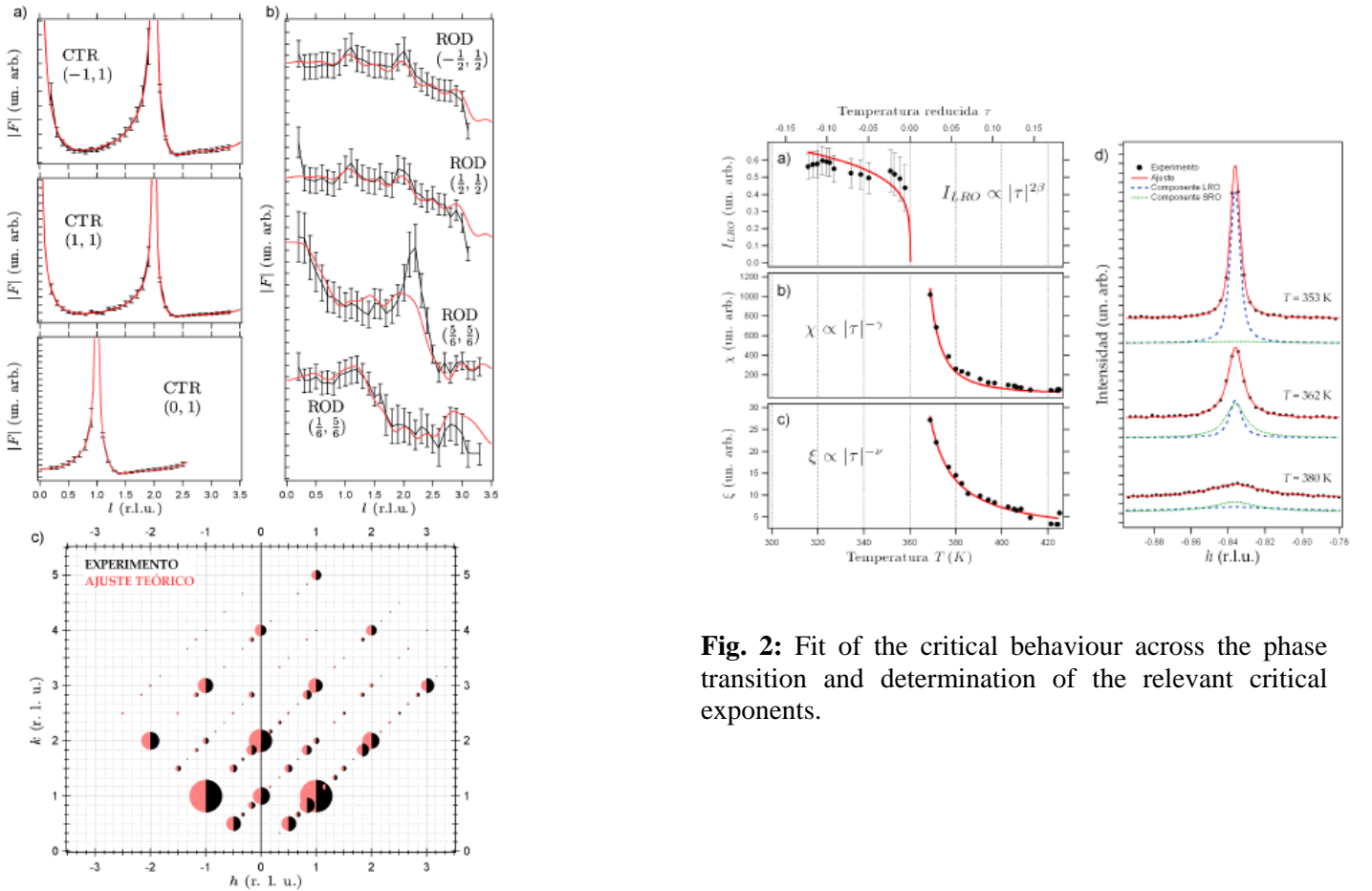
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**Report:**

We report an investigation on the structure of ISn on Cu(100) using surface x-ray diffraction. While the initial proposal dealt with the closely related In/Cu(100) interface, we decided to measure Sn/Cu(100) due to experimental difficulties in the evaporation of In. A  $p(3\sqrt{2}\times\sqrt{2})R45^\circ$  surface phase was obtained by Sn deposition on Cu(100) surface at room temperature followed by anneal. The formation of the phase was optimized by monitoring the intensity at the superstructure surface rods during the annealing process. Once a  $p(3\sqrt{2}\times\sqrt{2})R45^\circ$  reconstruction of satisfactory quality was obtained, we measured an ample data set in order to determine the crystallographic parameters of the reconstruction. To this end, crystal truncation rods (see Fig. 1), surface rods and in plane reflections were measured for both the RT  $p(3\sqrt{2}\times\sqrt{2})R45^\circ$  structure and the  $c(2\times 2)$  structure observed above  $360^\circ$  C. For the  $p(3\sqrt{2}\times\sqrt{2})R45^\circ$  structure, the data set includes 118 in-plane irreducible structure factor intensities and 122 out-of-plane irreducible structure factor intensities. In addition to this, 129 irreducible structure factors were measured for crystal truncation rods (CTR), providing a

total number of 389 structure factors. For the  $c(2 \times 2)$  structure, the data set includes 24 in-plane irreducible structure factor intensities and 183 out-of-plane irreducible structure factor intensities. In addition to this, 123 irreducible structure factors were measured for crystal truncation rods (CTR), providing a total number of 330 structure factors. The refinement of all the models includes horizontal and vertical displacements down to the fourth layer of the substrate and involves the use of a genetic algorithm implemented to be used along with the ROD code. The model developed used  $\sim 30$  independent parameters. This gives a rate of  $\sim 10$  experimental points per parameter. Several different models were considered to reproduce these data, in particular for the  $c(2 \times 2)$  structure. We conclude that the best model for the  $p(3\sqrt{2} \times \sqrt{2})R45^\circ$  is the Cu missing row model, in agreement with previous LEED data. For the  $c(2 \times 2)$  structure we obtain a description based on the disordering of the Cu missing row. The critical exponents of the phase transition have been determined also by fitting the critical behaviour of relevant superstructure peaks along the phase transition (Fig. 2). A detailed account of these results is under publication.



**Fig. 2:** Fit of the critical behaviour across the phase transition and determination of the relevant critical exponents.

**Fig. 1:** Integrated intensities of experimental CTRs rods, and in-plane structure factors (crosses and black half-circles) and fit to the data (red lines and half-circles)