	Experiment title: Structure of Br/Pt(110) along a charge density wave surface phase transition	**Experiment number**: SI-713
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Report:

We report an investigation on the structure of Br/Pt(110)-(3x1) using surface x-ray diffraction. A (3x1) surface phase was obtained by Br deposition on a Pt(110)-(2x1) surface at room temperature followed by anneal. The formation of the phase was optimized by monitoring the intensity at the x3 surface rods during the annealing process. Once a (3x1) 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. The data set includes 77 in-plane irreducible structure factor intensities and 120 out-of-plane irreducible structure factor intensities. In addition to this, 120 irreducible structure factors were measured for crystal truncation rods (CTR), providing a total number of 317 structure factors.. The refinement of all the models includes horizontal and vertical displacements down to the third layer of the substrate. The models developed used ~30 independent parameters. This gives a rate of ~10 experimental points per parameter.. Several different models were considered to reproduce these data. the (3x1) . We considered first substitutional models, that were discarded due to an

overall poor agreement. Next, adsorption models were considered, with on top, long bridge, hollow, and short bridge sites, as well as suitable combinations of them in an effort to reproduce previous STM and LEED results. We conclude that the best model is obtained with by Br atoms at the short bridge sites, with an additional Br atom at a long bridge site (see Fig. 2). A detailed account of these results is under publication.

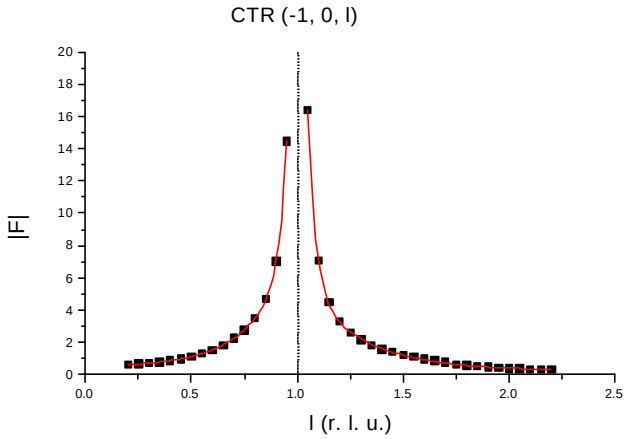

Fig. 1: Integrated intensities of experimental (-1,0,l) CTR (points) and fit to the data (lines).

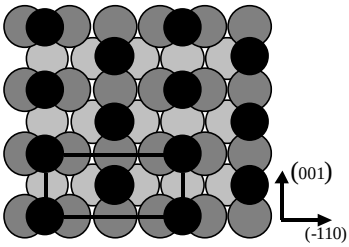

Fig. 2: Side view of the structural models found for Br/Pt(110)-(3x1). Black circles denote Br atoms, light and dark grey circles denote Pt atoms in the second and first atomic layers, respectively.