	Experiment title: **Role of the electronic structure in the surface relaxation of Au(111)**	**Experiment number**: 25-02-809
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Report:

We report an investigation on the surface relaxation of Au(111) using surface x-ray diffraction. The aimed to establish a relationship between the surface relaxation of Au(111) covered with adsorbates and the concomitant filling/emptying of the surface state, induced by the adsorbates.

This Proposal was the continuation of a previous one (25-02-778) where preliminary results pointing towards the observation of the effect were obtained. The experiments ran very well and we obtained satisfactory results that demonstrate the effect for charge donors, i.e. when the amount of charge at the surface state is increased. We prepared successfully a Au(111) surface. The pristine Au(111) surface is characterized by a long-range reconstruction with a complex atomic arrangement ("herringbone"). We observed superstructure spots in grazing incidence SXRD and used their intensity to monitor the surface quality. Next, we deposited K atoms as charge donors. The interactions and surface structure of K/Au(111) are well known and had been tested by us in our home laboratory. For a coverage of 0.33 ML a ($\sqrt{3}$x$\sqrt{3}$)R30º reconstruction is formed. We used the formation of this superstructure, and the appearance of the corresponding superstructure x-ray reflections, as a way to calibrate K coverage. Indeed, we were interested in the low K coverage range, when charge donation per K atom is largest.

In this coverage range we expected that the direct structural effect of K adsorption is minimal, so that structural changes in the Au(111) relaxation can be safely attributed to the change in charge contained in the Au(111) surface state.

In order to monitor the surface relaxation we measured several different Au(111) CTRs for the Au(111) clean surface and for several K coverages in the submonolayer range. We developed a complex model, based on the crystallographic properties of the Au(111) surface with a herringbone reconstruction. The experimental results were fitted using this model and we reached an excellent agreement in the fitting process. The analysis made correlates the surface expansion with the intensity increase of the minimum of the (0 1 L) CTR observed in the experiment, and quantifies the amount of the expansion. A theoretical calculation is being performed in order to shed light in the mechanisms of the surface relaxation. The results will be published soon.