



Experiment title: Role of the electronic structure in the surface relaxation of Cu(111)

Experiment number:
25-02-778

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Report:

We report an investigation on the surface relaxation of Au(111) using surface x-ray diffraction. The main goal of the proposal was to establish a relationship between the anomalous surface relaxation of some well know surfaces and the amount of electronic charge contained in their surface states. To this end, we proposed to investigate the change in surface relaxation of (111)-oriented noble metal surfaces, which present a conspicuous surface state band, upon depositing adequate charge donor and acceptor species. The experiments ran well and we have 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 know and had been tested by us in our home laboratory. For a coverage of 0.33 ML a $(\sqrt{3} \times \sqrt{3})R30^\circ$ 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 are interested in the low K coverage range, when

charge donation per K atom is largest, and when we foresee 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. Fig.1 shows a selection of the results after a preliminary integration of the data (note that the beamtime finished a few days before this report was submitted). There is a intensity change upon K adsorption near the CTR minimum. The shift is large for 0.33 ML (corresponding to the $(\sqrt{3}\times\sqrt{3})R30^\circ$ reconstruction), but there is also a significant shift for a much smaller K coverage. This is a promising result and we are currently working in a detailed analysis of the data.

Unfortunately, due to the limited beamtime available we could not use charge acceptors to prove an opposite shift of the relaxation and to demonstrate that the amount of charge controls the surface structure.

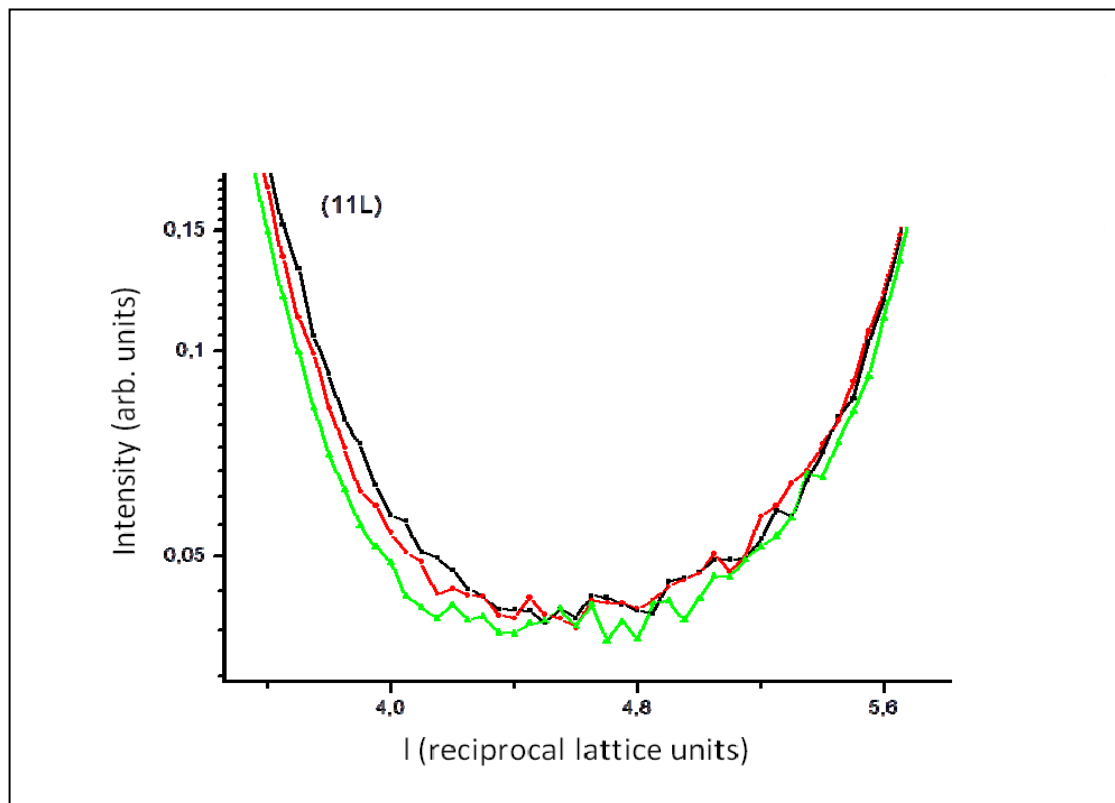


Fig. 1 (11L) CTRs as a function of K coverage: clean Au(111) (black), ~ 0.05 ML (red) and 0.33 ML (green). Note the small intensity change for low K coverage.