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# The role of surface states in the Na/Cu(110)(1 × 2) reconstruction

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## Abstract

Reflection anisotropy spectroscopy (RAS) is combined with scanning tunnelling microscopy in a study of the Na/Cu(110)(1 × 2) surface reconstruction induced on the thermally roughened Cu(110) surface. The roughening transition of Cu(110) generates a surface morphology consisting of a high density of exclusively monatomic height steps. This surface is further characterized by the irreversible loss of the 2.1 eV RAS feature and an enhancement in the response around 4 eV. Na deposition onto the roughened surface results in the formation of the (1 × 2) reconstruction. We show that the occupancy of the surface state near the Fermi level at  $\bar{Y}$  on Cu(110) is not a prerequisite for surface reconstruction.

## 1. Introduction

The localization of surface electronic states at the outermost layers of metal single crystals makes them sensitive to a variety of surface phenomena, including adsorption and structural changes on the atomic scale [1]. The Cu(110) surface has two surface states located in the bulk band gap that exists in the region of the Fermi level ( $E_F$ ) at the  $\bar{Y}$  point of the surface Brillouin zone. At room temperature, one surface state is located at an energy 0.4 eV below  $E_F$  [2] and the other at 1.8 eV above  $E_F$  [3]. The response of these surface states to the formation of the Na/Cu(110)(1 × 2) surface reconstruction has been studied by photoemission and inverse photoemission [4]. The surface states shift in energy and experience charge depopulation upon reconstruction [4] and it has been argued that they contribute significantly to the total energy balance of the adsorbate induced reconstruction [5]. In our work reported here, we show that the occupancy of the surface state is not a prerequisite for the Na/Cu(110)(1 × 2) reconstruction.

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The optical technique of reflection anisotropy spectroscopy (RAS) is a probe of the surface electronic structure of cubic metal crystals around the Fermi level ( $E_F$ ) [6] and has been shown to be sensitive to transitions involving surface states [7–10]. RAS uses linearly polarized light to probe, as a function of energy, the difference in normal incidence reflection of two perpendicular directions ( $\Delta r$ ) normalized to the mean reflection ( $r$ ):

$$\frac{\Delta r}{r} = 2 \left( \frac{r_{[1\bar{1}0]} - r_{[001]}}{r_{[1\bar{1}0]} + r_{[001]}} \right)$$

where  $r$  denotes complex Fresnel reflection amplitudes.

The Cu(110) surface has been the subject of a number of RAS studies and significant progress has been made in the interpretation of the Cu(110) RA spectrum. It has been established that the RA peak observed at 2.1 eV arises from two different contributions. The dominant contribution originates from transitions between the two surface states at the  $\bar{Y}$  point [7, 11, 12]. The second contribution to the RA signal has been assigned [13, 14] to local-field effects at the surface and can be modelled using the surface local-field model developed in [15]. The behaviour of the 2.1 eV peak in the RA spectrum following the Na induced Cu(110)(1 × 2) reconstruction has been found to be consistent with the known behaviour of the surface states at  $\bar{Y}$  [12]. In particular, the intensity of the 2.1 eV peak was found to decrease as the various phases of the reconstruction proceeded.

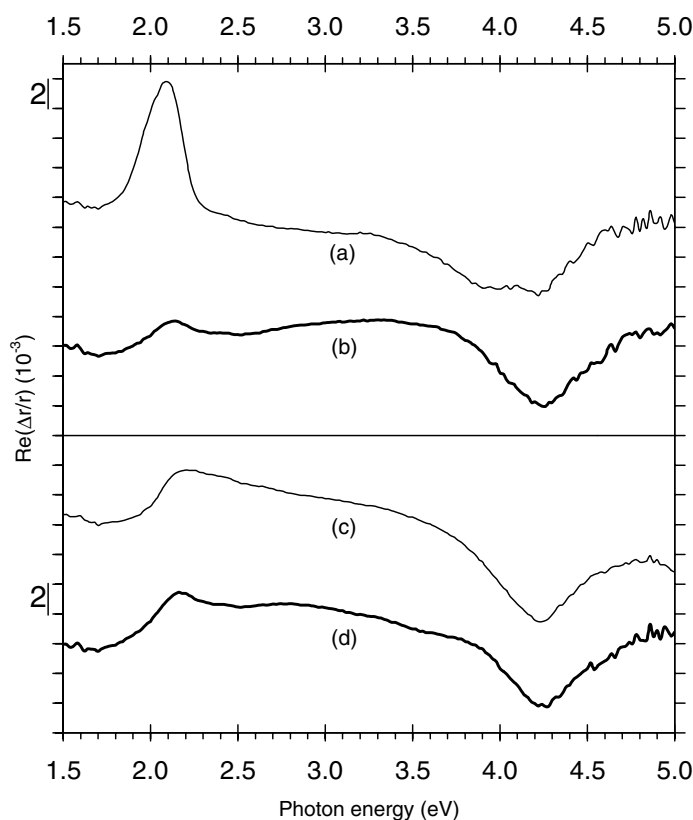
In a recent study, we reported RAS and scanning tunnelling microscopy (STM) results of the thermally roughened Cu(110) surface [14]. At a temperature of approximately 1000 K, the roughening transition occurs, characterized by the proliferation of [001] oriented monatomic steps across the surface creating a well-defined surface morphology. The RAS results from this surface show an absence of the 2.1 eV peak [14], indicating that this surface has no electrons in the surface state at  $\bar{Y}$ . To investigate further the role of surface states in the process of reconstruction, the roughened surface characterized by the array of monatomic [001] steps was used as a substrate for Na deposition.

## 2. Experimental

The experiments were carried out in an ultra-high vacuum environment with a base pressure in the  $10^{-11}$  mbar region. The mechanically polished Cu(110) single crystal aligned using Laue x-ray diffraction to  $0.5^\circ$  was introduced into the vacuum chamber and a clean Cu(110) surface was prepared by cycles of Ar ion bombardment ( $10 \mu\text{A cm}^{-2}$ , 0.5 kV, 300 K, 20 min) and subsequent annealing to 850 K. Surface order was confirmed by a sharp (1 × 1) low-energy electron diffraction (LEED) pattern and cleanliness was monitored using x-ray photoelectron spectroscopy (XPS). The roughened Cu(110) surface was prepared by annealing the clean surface to  $\sim 1060$  K and the specimen held at this temperature for 15 min.

Na was deposited at room temperature from a fully outgassed commercially available dispenser. Coverage was determined from the relative intensities of the Na 1s and Cu 2p core-level photoelectron lines and by LEED analysis [16–18]. We define Na coverage as the ratio of Na atoms to Cu atoms in the unreconstructed surface layer, i.e. one monolayer (ML) corresponds to  $1.1 \times 10^{15}$  Na atoms  $\text{cm}^{-2}$ . The Na/Cu(110)(1 × 2) surfaces were prepared by deposition of 0.6 ML.

*In situ* STM was performed at room temperature in constant current mode using a tunnelling current of 1 nA and bias voltage  $-1.0$  V. The STM tip was made from tungsten wire electrochemically etched and prepared *in situ* by annealing. The RA spectrometer of the Aspnes design [19] projected and received light through a low-strain window on the UHV system. Experimental artefacts were removed from the spectra using a correction function



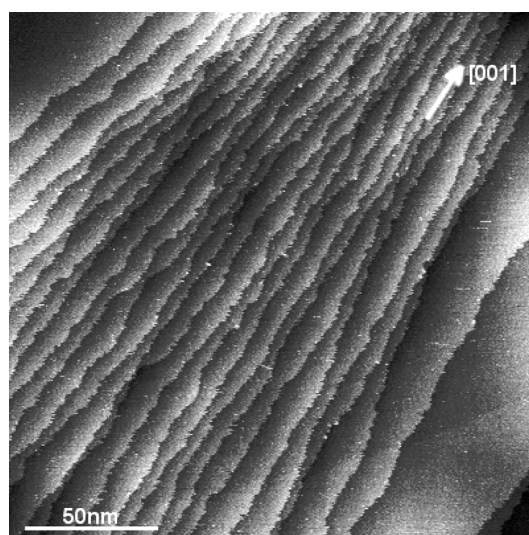
**Figure 1.** RA spectra. Upper panel: the RA profile of the clean Cu(110) surface prepared by bombardment and anneal cycles (a) and the result of Na deposition (b). Lower panel: the RA profile of the thermally roughened Cu(110) surface (c) and the result of Na deposition (d).

obtained by measuring spectra with the sample in two orthogonal positions. Spectra of the real part of the complex RA were taken over a photon energy range of 1.5–5.0 eV. RAS and STM data were taken with the specimen at room temperature.

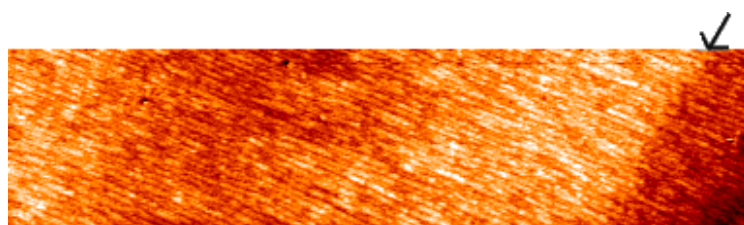
### 3. Results

The upper panel of figure 1 shows RA spectra of the clean Cu(110) surface (curve (a)) and the Na/Cu(110)(1 × 2) surface (curve (b)), both obtained from the Cu(110) surface prepared by standard Ar ion bombardment and annealing cycles. Plotted in the lower panel of the figure are RA spectra of the thermally roughened Cu(110) surface (curve (c)) and the Na/Cu(110)(1 × 2) surface (curve (d)) prepared from the roughened Cu(110) surface.

The spectral profile of the roughened Cu(110) surface (curve (c)) does not exhibit the intense peak at energy 2.1 eV and the doublet structure around 4 eV that are the main characteristics of the surface prepared by conventional methods (curve (a)). In a previous study [14] we attributed the changes induced in the RA profile by roughening the surface to two effects. The loss of the peak at 2.1 eV is due to charge depopulation of the occupied surface state at  $\bar{Y}$  and the residual structure in the RA response around 2 eV is assigned to the surface local-field effect. The enhanced RA response at 4 eV on the roughened surface is attributed



(a)



(b)

**Figure 2.** STM data. (a) The thermally roughened Cu(110) surface. (b) The Na/Cu(110)(1 × 2) reconstructed surface obtained on the roughened surface, showing the  $[1\bar{1}0]$  rows of the reconstruction and the reduced density of [001] steps (arrows). Image (b) has the same orientation as image (a).

(This figure is in colour only in the electronic version)

to the surface morphology that STM results show to consist of an array of [001] oriented steps terminating narrow terraces (figure 2(a)). The STM results for the roughened Cu(110) surface following Na deposition show considerable changes to the roughened morphology. Before deposition the roughened surface consists of narrow terraces, typically 5–15 nm wide, separated by monatomic [001] steps (figure 2(a)). After deposition there are far fewer steps (approximately an order of magnitude less are observed over equivalent areas) that are of single and double atomic height and towards [001] orientation (figure 2(b)). The terrace widths have significantly increased, up to 150 nm (figure 2(b)). The reconstructed surface shows regions of (1 × 2) and (1 × 3) phases with the Na adatom rows imaged as troughs, in agreement with previous STM studies [20].

The RA profile obtained following Na deposition on the roughened surface (curve (d)) is very similar to that obtained by deposition on the surface prepared by conventional cleaning methods (curve (b)).

#### 4. Discussion

The Na induced (1 × 2) reconstruction at coverage of 0.6 ML involves missing rows of Cu atoms in the  $[1\bar{1}0]$  direction (figure 2(b)). The Cu missing rows are occupied by rows of Na atoms located in sites that are randomly out of phase with each other [18]. Our *in situ* STM studies of the roughened Cu(110) surface show that the deposition of Na significantly increased the width of terraces and produces a corresponding reduction in the number of [001] monatomic steps (figure 2(b)). Following reconstruction of the roughened surface a small but notable change was observed in the shoulder in the RA spectrum at 2.2 eV, together with a significant reduction in intensity of the feature observed at 4.2 eV (figures 1(c) and (d)). The latter reduction of intensity is consistent with the assignment of the 4.2 eV RA feature to the contribution from monatomic [001] steps and the reduction in the number of these steps following the reconstruction.

The key observation is that, for the same Na coverage, the Na induced (1 × 2) reconstruction of the roughened surface gave rise to an RA spectrum (figure 1(d)) similar to that observed from the Na induced (1 × 2) reconstruction of the surface produced by Ar ion bombardment and annealing treatments (figure 1(b)). This observation shows that the (1 × 2) reconstruction will occur whether or not the surface state that is the initial state for the 2.1 eV RAS transition is occupied, as shown by the presence of the intense 2.1 eV peak in the RA spectrum shown in figure 1(a), or unoccupied, as shown by the absence of this peak from the RA spectrum of figure 1(c). The occupation of this surface state is not then an essential prerequisite for the reconstruction process.

#### 5. Conclusions

Irreversible changes to the RA spectrum of Cu(110) are observed upon inducing the roughening transition that are related to the surface state occupancy and the response from monatomic steps. We have shown that the formation of the Na/Cu(110)(1 × 2) reconstruction does not require the surface state at  $\bar{Y}$  on the clean Cu(110) surface to be occupied.

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