Comment on "Oxygen Chemisorption on Cu(110): An Atomic View by Scanning Tunneling Microscopy"

In a recent scanning-tunneling-microscopy (STM) study of the (2×1)-O/Cu(110) system, Chua, Kuk, and Silverman[1] suggested a buckling of every second outermost ⟨100⟩ Cu row. This is in clear contrast to surface-extended x-ray-absorption fine-structure-spectroscopy (SEXAFS) results[2] which indicate that every second ⟨100⟩ Cu row is missing. The STM data are interpreted as suggesting that the "O-induced rows" are vertically displaced by 0.8 ± 0.2 Å from the "truncated bulk" position [cf. inset in Fig. 1(b)]. Chua, Kuk, and Silverman then take our earlier SEXAFS values[3] for the nearest- and second-nearest-neighbor O-Cu distances and derive a structural model in which the oxygen is located 0.35 Å below the level of the buckled Cu atoms (or 0.45 Å above the truncated bulk position of the outermost Cu layer). The more recent SEXAFS data taken under improved experimental conditions[2] (and not considered by Chua, Kuk, and Silverman) have since confirmed the earlier bond-length determinations *and* have clearly indicated that the reconstruction is of the missing-row type.

Figure 1(a) shows the Fourier transform of the SEXAFS spectrum taken at normal x-ray incidence in the ⟨110⟩ azimuth.[2] Second- (R_2=1.99 Å) and fourth- (R_4=4.15 Å) nearest-neighbor distances are evident, whereas a Fourier peak for the third-nearest-neighbor distance R_3 (which would occur for an unreconstructed or buckled Cu surface) is clearly missing. Figure 1(b) shows Fourier transforms of SEXAFS simulations for the structural model proposed in the STM study (dotted line) and for an oxygen-covered surface which is reconstructed according to the missing-row model[2] (solid line). The amplitude of an R_3 feature would be relatively independent of the position of the oxygen atom: If the possible outward displacement of the second Cu layer is limited to 20% of the bulk interlayer spacing (which already seems unrealistically large), the SEXAFS bond lengths[2] are compatible with an oxygen location in the STM model between 0.20 and 0.53 Å above the truncated bulk position of the outermost Cu layer. This corresponds to an amplitude for R_3 which is between 80% and 90% of the R_2 amplitude. The calculations in Fig. 1(b) assume a constant Debye-Waller factor (DWF). Even if there is a considerable R dependence in the DWF, the amplitude of the third-nearest-neighbor peak is reduced by less than 25%.

We suspect that the reason for the discrepancy lies in the interpretation of the STM data. An STM topograph basically reflects the density distribution of electrons near E_F about 10 Å in front of the surface, which makes a determination of the exact atomic geometry on an adsorbate-covered surface extremely difficult. Particularly on oxygen-covered surfaces electronic effects are known to lead to considerable deviations of the STM topograph from the surface geometry, in agreement with theoretical considerations.[4]

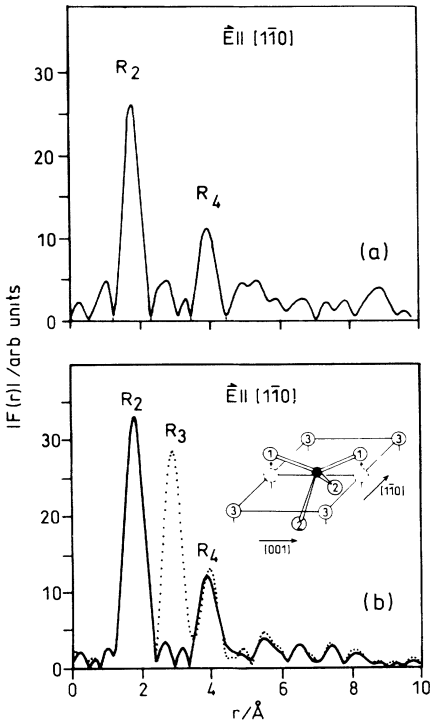

FIG. 1. (a) Fourier transform of the experimental SEXAFS spectrum for (2×1)-O/Cu(110) taken with E∥[1$\bar{1}$0] (Ref. 2). (b) Fourier transforms of calculated SEXAFS spectra for E∥[1$\bar{1}$0] according to the missing-row reconstruction (Ref. 2) (solid line) and the buckled-row model proposed in the STM study (Ref. 1) (dotted line). Inset: The latter model with the numbers referring to the first-, second-, and third-nearest Cu neighbors of the adsorbed oxygen atom (circles).

In summary, the SEXAFS data are only compatible with the missing-row model for the reconstruction of the (2×1)-O/Cu(110) system. The buckled-row model proposed as a result of the STM study must be excluded. Incidentally, the same holds for a structural model in which the non-oxygen-containing [001] Cu rows are elevated.

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