Intricate Mechanism of Lateral and Vertical Manipulation of Super-Cu Atoms on the Cu:O Surface: Experiment and Theory

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We present a join experimental and theoretical study of lateral and vertical manipulations of "super"-Cu atoms on the oxygen-terminated p(2x1) Cu(110) surface with Non-Contact Atomic Force Microscopy (NC-AFM). The surface consists of rows of alternating Cu and O atoms on the bare Cu(110) surface. Cu adatoms occupy positions between two adjacent Cu-O rows opposite two O atoms in each of them. Using NC-AFM we find that using an O terminated tip [1] vertical manipulation events, consisting of both removal and deposition of Cu atoms, are frequently seen, Fig. 1 (right). Interestingly, no change of contrast is observed. At the same time, lateral manipulation events were observed only at the edges of c(6x2) islands, no lateral manipulation was found to be possible on the p(2x1) terraces.

In order to understand these observations, we attempted a comprehensive theoretical study of both lateral and vertical manipulations of the super-Cu atoms on the p(2x1) Cu(110):O surface with the O-terminated NC-AFM tip. Using Density Functional Theory (DFT) calculations in conjunction with Nudged Elastic Band (NEB) method for calculating transition barriers, as well as Kinetic Monte Carlo (KMC) simulations, we propose detailed mechanisms of both lateral and vertical manipulations, which fully explain experimental observations. We find that both mechanisms depend crucially on the initial tip-surface separation. At not very small separations a super-Cu atom under the tip (state S) can be thermally activated into an intermediate (I) position between the tip and surface, Fig. 1 (left). Upon tip retraction, the atom remains in this state until the barrier to jump to the tip (state T) is sufficiently reduced. Upon reaching state T, however, the Cu atom immediately moves higher up on the tip (state U), so that tip apex remains O-terminated with only secondary features in the imaging contrast affected. The deposition of the Cu atom from the tip to the surface happens when the barrier for the atom from U to T state is reduced which happens at smaller separations. Therefore, the mechanism consists of several stages: three stochastic (thermal with en energy barrier) and one conservative (dragging), which happen in between. KMC simulations confirm the viability of this mechanism and give statistics information.

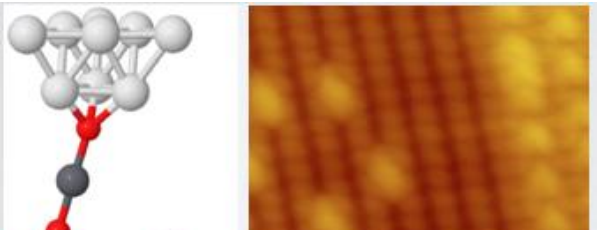

Figure 1 Intermediate state of the Cu atom (left) and the NC-AFM image during manipulation (right) with super-Cu atoms clearly visible on the terrace (central area) alongside some vertical manipulation events. The edge of the c(6x2) island is seen in the right part of the image.

We find that lateral manipulation (based on a certain deviation of the above mechanism) can only be rationalized if the tip comes much closer to the surface, which explains why these particular events were not frequently observed.

[1] J. Bamidele et al. – Phys. Rev. B **86** (2012) 155422.