Controlled manipulation of adatoms on the Oxidized p(2x1) Cu(110) surface using NC-AFM

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We have shown previously [1] that it is currently possible to control the chemical termination of the NC-AFM tip when scanning the oxidised c(6x2) reconstructed Cu(110) surface as clear difference in the imaging pattern is observed when the tip is terminated either with O, Cu or Si atoms. This allows one to employ this particular surface as a reference system for NC-AFM imaging. Most importantly, the tip termination can be checked before and after performing an atomic manipulation (by imaging), and hence would be known, which is absolutely essential for understanding the manipulation mechanism at hand.

Experimentally, large finite regions (islands) of the c(6x2) reconstruction bordering (also rather substantial) regions of the p(2x1) reconstruction with single super-Cu atoms between some neighbouring -Cu-O-Cu- rows can be created on the oxidised Cu(110) surface, see Fig. 1A. Here we report on our combined theoretical and experimental study of the manipulation of these isolated super-Cu atoms with NC-AFM.

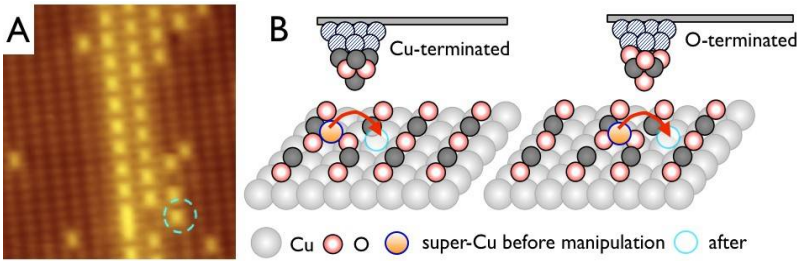

Figure 1. (A) AFM image of a c(6x2) island (centre); individual super-Cu atoms on the p(2x1) regions next to it are seen mostly on the left. (B) Schematics of the manipulation.

Theoretical calculations were performed using the density functional theory (with particular attention paid towards including non-local correlation effects), as implemented in the VASP code. Two Cu tip models were used [1] terminated either with Cu or O atoms. Placing either of the two tips at various positions around the super-Cu atom on the surface, we calculated maps of the corresponding energy barriers for the transition of the super-Cu atom to the neighbouring site (see Fig. 1B) with the help of the Nudged Elastic Band (NEB) method. Using these comprehensive data and the virtual AFM (vAFM), mimicking the actual NC AFM apparatus, we modelled the manipulation mechanism and obtained the corresponding tip response during the individual manipulation events. These were compared with available experimental results on the atomic manipulation.

[1] J. Bamidele et al. – Phys. Rev. Lett. 2012 (under review).