

Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Controlled manipulation of adatoms on the oxidized $p(2 \times 1)$ Cu(110) surface using NC-AFM JOSEPH BAMIDELE, Dept. of Physics, King's College London, U.K., ROBERT TURANSKY, Inst. of Physics, Slovak Acad. of Sciences, 84511 Bratislava, Slovakia, YASUHIRO SUGAWARA, Dept. of Applied Physics, Osaka University, Japan, IVAN STICH, Inst. of Physics, Slovak Acad. of Sciences, 84511 Bratislava, Slovakia, LEV KANTOROVITCH, Dept. of Physics, King's College London, U.K. — Experimentally, large finite regions (islands) of the $c(6 \times 2)$ reconstruction bordering (also rather substantial) regions of the $p(2 \times 1)$ reconstruction with single super-Cu atoms between some neighboring -Cu-O-Cu- rows can be created on the oxidized Cu(110) surface. We report on our combined theoretical and experimental study of the manipulation of these isolated super-Cu atoms with NC-AFM. Experiments indicate that the manipulation proceeds mostly by vertical manipulation with a small number of lateral manipulation events. Theoretical calculations were performed using the density functional theory (with particular attention paid towards including non-local correlation effects). Two Cu tip models were used 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 neighboring site and/or for tip adsorption and desorption. Using these comprehensive data and the virtual AFM, mimicking the actual NC AFM apparatus, we modeled the manipulation mechanism and obtained the corresponding tip response during the individual manipulation events.

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Date submitted: 10 Dec 2012

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