

RESOLUTION OF THE SURFACE STRUCTURE OF AN OXIDE FILM ON AG(111) FROM THE INTERPLAY BETWEEN MEASURED AND CALCULATED STM IMAGES.

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Abstract :

The STM technique doesn't give an atomic topographic view of a conducting surface but is very sensitive to the electronic structure and coordination of the surface atoms. For complex systems like the one presented here, where lots of outer atoms (either O or Ag) are facing the tip and only part of them yield an atomic current corrugation, the simulation of the STM high-resolution image can be very helpful.

I will first briefly describe the simulation method which stems from a diffusion formalism to handle the tunnel junction. I will then point out the chemical approximations for the current calculation but also the advantages of the method compared to an usual Tersoff-Hamman approach.

In a second part, I will present high resolution images of the vacuum-oxide surface atomic structure which reveal large terraces of perfect (4x4) reconstruction. Under certain conditions, these STM experiments have been able to provide the structural registry between the reconstructed oxide layer and the underlying Ag(111) lattice.

In a third part, the proposed structural results arising from a combined experiment-simulation approach will be analyzed [1]. Finally, I will show that the key point to retrieve the experimental image, is to position a 4x4 array of Ag vacancies in the trilayer oxide, while the precised feature of the image is controlled by a buckling between two chemical types of outer Ag atoms.

[1] C.I. Carlisle, D.A. King , M.-L. Bocquet, J. Cerdà and P. Sautet, PRL **84**, 3899 (2000).