

NC-AFM imaging of Au clusters on the KBr surface

O. H. Pakarinen*, C. Barth**, A. S. Foster*, R. M. Nieminen* and C. Henry**

*Laboratory of Physics, Helsinki University of Technology, P. O. Box 1100, Helsinki 02015, Finland

**CRMC2-CNRS, Campus de Luminy, case 913, 13288 MARSEILLE Cedex 09, France

Small gold clusters have received significant interest lately due to the observation that Au, an inert material in the bulk form, shows significant catalytic activity when it is in the form of small clusters adsorbed on insulating surfaces. An ideal experimental study of these clusters would image both the cluster and the surface in atomic resolution - thereby providing great detail on their properties. Noncontact atomic force microscopy (NC-AFM) is the obvious tool for this investigation, and here we combine atomically resolved experimental images with first principles simulations to attempt to provide a comprehensive picture of the system.

Experimental NC-AFM images of Au clusters on KBr demonstrate high quality atomic resolution of the insulating substrate, but no resolution on the clusters themselves. Images show resolution even in-between closely spaced clusters, indicating that the effect is not due to tip-convolution. Initially, we consider some idealized small Au clusters on the surface as models for the very large (several nms) clusters observed in experiment. We then calculate the interaction of both a KBr and a Au contaminated tip with the clusters and the KBr surface, and compare our results to experimental observations.

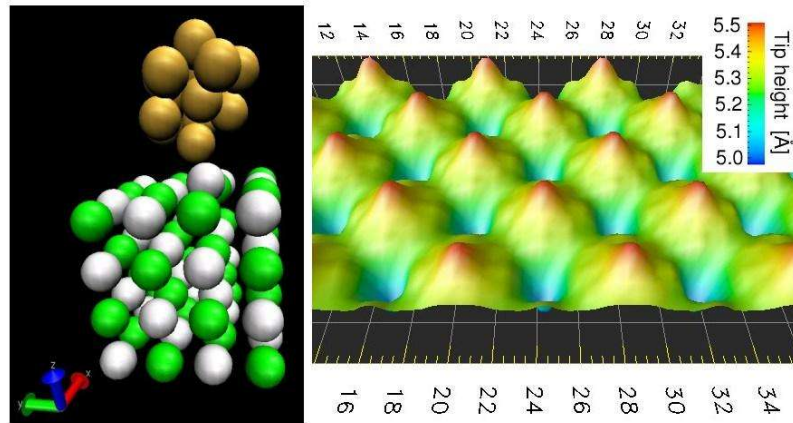


Illustration 1(a) Simulation snapshot of gold tip scanning KBr surface. (b) Simulated image of the KBr surface with a KBr tip.

Results from the NC-AFM scanning simulations of the KBr(001) surface, using the same tips and experimental scan parameters, result in simulated topographic images with good agreement with experimental images. The NC-AFM scan simulations using K^+ - and Br^- -terminated $(KBr)_6$ tips and a Au_{13} tip show that the difficulties in imaging Au clusters are probably due to the strong deformations seen already at quite large tip-surface separations. Scanning of the gold clusters on the surface are then simulated using a Au_{27} cluster, flat enough to represent a much larger surface cluster.