Imaging and Manipulation of Single Atoms on the Si(111)-(7x7) Surface

P. Jelinek[1,2], P. Pou Bell[1], N. Oyabu[3], M. Abe[3], O. Custance[3], S. Morita[3] and R. Pérez[1]
[1]Dpto. de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, Spain.
[2]Institute of Physics, Academy of Sciences of the Czech Republic, Prague, Czech Republic.
[3]Graduate school of Engineering, Osaka University, Japan.
ruben.perez@uam.es

A detailed knowledge of the short-range tip-sample interactions is the key ingredient for the understanding of the experimental topographical and damping images obtained with the Noncontact Atomic Force Microscope. While image contrast, corrugations and force-distance curves on semiconductors in the attractive regime can be explained in terms of the interaction between the surface unsaturated bonds with the dangling bond of a simple reactive tips, recent experimental evidence[1], that explores in detail the repulsive regime, suggests that a more realistic description of the mechanical properties of the tip is needed in order to understand quantitatively the near-contact region. To this end, we have explored the structure and mechanical properties of different large tips, generated from initial configurations with (111) and (001) orientations with different procedures, that include ab initio molecular dynamics annealing and the breaking of thick nanowires subject to tensile strain[2-4]. Using the most stable resulting tips, we perform different lateral scans and approach curves on different positions of the Si(111)-7x7 unit cell in order to understand (1) the contrast between different adatoms observed in the topographical and damping images and (2) The atomistic mechanism behind the vertical manipulation of adatoms with the NCAFM.

[1] N. Oyabu, O. Custance, I. Yi, Y. Sugawara and S. Morita, Phys. Rev. Lett., **90**, 176102 (2003)
[2] P. Jelinek, R. Perez, J. Ortega and F. Flores, Phys. Rev. B 68, 085403 (2003).
[3] P. Jelinek, R. Perez, J. Ortega and F. Flores, Surf. Sci. 566-568, 13 (2004).
[4] P. Jelinek, R. Perez, J. Ortega and F. Flores, Nanotechnology (in press, 2005).