Surface atoms and the AFM tip: Simulation of scans for GaAs(110) and Si(100)

V.Bus and J.Redinger
Inst. f. Allgemeine. Physik and Center for Computational Materials Science
Vienna University of Technology, Getreidemarkt 9/134, A-1060 Wien
E-mail: vb@cms.tuwien.ac.at, jr@cms.tuwien.ac.at

Non-contact Atomic Force Microscopy – (nc-AFM) is a technique capable of true atomic resolution on non-conducting surfaces. Forces due to tip-sample interactions cause changes in the measured frequency of ab AFM tip oscillating above the surface. Electrostatic and van der Waals interactions lead to a long range or background contribution. Short range or chemical forces are involved in the very proximity. The on-set of covalent bonding between the tip apex atom and the respective surface atom is responsible for SFM contrast formation, e.g. on semiconductor surfaces. For small oscillation amplitudes, chemical forces overshadow the other contributions, which are neglected in simulations of such systems and play a crucial role in contrast formation, as already mentioned.

Recently, DFT methods were implemented to simulate rigorously what happens when the oscillating tip of the SFM cantilever approaches the surface to a maximum proximity. Recent DFT calculations show the onset of covalent bonding and mutually induced tip-sample reconstruction (local distortions) [1-3]. GaAs(110) and Si(100) surfaces were chosen as a starting point for our calculations. Both surfaces share a common feature in their topmost layers. Both the Si(100) buckled-dimer reconstruction and the GaAs(110) buckling yield a higher (up) and a lower position (down) for the surface atoms, for which a difference in tip-sample interactions is to be expected..

Our model calculations employ the DFT VASP code [4] (Vienna Ab-initio Simulation Package) in its PAW incarnation and using the PW91-GGA. SFM probing over the GaAs(110) surface was modeled in a repeated slab geometry supercell consisting of 6 GaAs(110) planes. A mesh of 4 irreducible k-points and a cut-off energy of 245 eV was used. The top-most layer was fully relaxed and shows a buckling of As outwards and Ga inwards as depicted in Fig.1. Into the separating vacuum region between the GaAs slabs a model tip was inserted, consisting of 4 (tetrahedron) Si atoms and three hydrogen atoms to saturate the dangling bonds.

We start the tip approach towards the surface at a distance of 5 Å measured between the apex atom of the tip and the surface As atom. During the calculation the tip apex atom and the topmost layer slab atoms were let to relax and to find their minimum positions.. As shown in Figs. 2 and 3, an almost “classical” set of data for the interaction energy and the tip forces with respect to tip-sample distance was obtained for the tip above the As atom. The situation for a tip above a Ga atom is very different. An abrupt change in energy and lateral force was observed. A hysteresis loop obtained between approach and removal of the tip signals the difference between the formation and the breaking-up of the Si-tip-Ga-surface-atom system, after which the tip remains slightly distorted.

Concerning the Si(100) surface, the same computational procedure as for the GaAs surface was applied. A scan above an higher Si buckled-dimer atom did not reveal anything unexpected. For the lower Si buckled-dimer atom, however, similar to the Ga atom of a GaAs surface, the dimer starts to tilt and the Si tip apex atom and the lower dimer atom snap together during the approaching move shown in Fig. 4. On withdrawal, the dimer does not seem to return to its original position. Such a behaviour is supported by experiments, which indicate that at finite temperatures the dimers eagerly tend to change their tilt angle considerably, and when averaging in time, they are sometimes even considered as flat.

References

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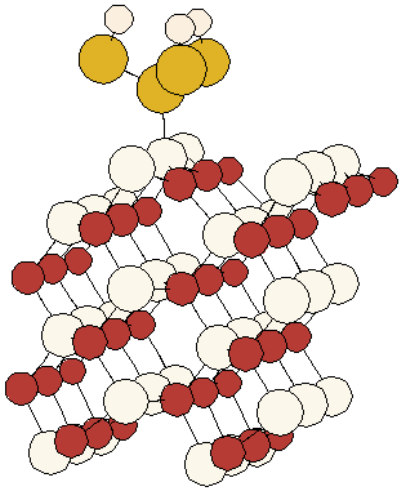


Fig. 1. Si tip above As on a GaAs(110) surface. 79 atoms make up the model system.

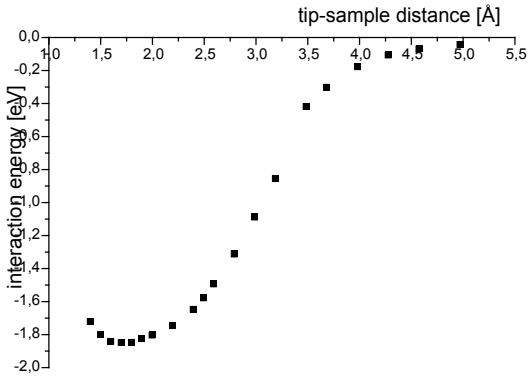


Fig. 2. Interaction energy between the tip and GaAs(110) surface approaching an As atom

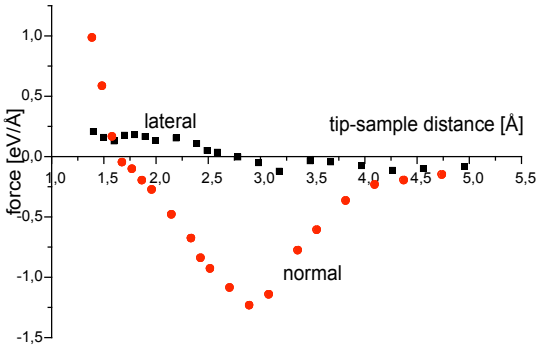
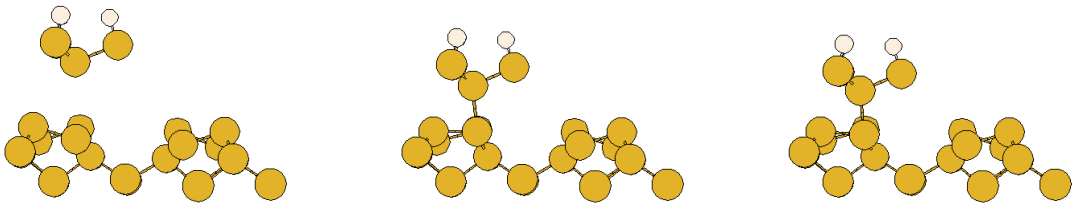


Fig. 3. Normal and lateral force on the tip



a b c

Fig. 4. Tip above a lower Si buckled-dimer atom at distances of 3.7 Å (a), 2.55 Å (b), and 1.6 Å (c) demonstrating the "flexibility" of the buckled-dimer.