Different contrasts in atomically resolved scanning force microscopy images of Si(111) 7x7

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Abstract

Among scanning probe microscopies, scanning force microscopy (SFM), in particular in its dynamic mode under the frequency-modulation detection method (FM-DSFM), has shown to be a powerful tool for investigating the topography of both, conducting and insulating surfaces, at the nanometer scale. Owing to the high degree of complexity of the FM-DSFM instrumentation, atomic resolution was only obtained around ten years after its invention. For resolving atoms with the SFM microscope, the short-range forces related with the interaction of the foremost atom at the end of the cantilever and the atoms at the surface have to be detected [1,2]. These forces depend on the chemical and physical nature of both the tip apex and of the nearby sample atoms [3], and become appreciable at very close distances between the tip and the surface (typically <5 A). But the chemical and physical nature of the tip of the cantilever is often modified during the experiment (crashes, picking or losing atoms), making complicated the interpretation of the images obtained [3]. Additionally, long-range forces are also present, in vacuum they mainly correspond to the van der Waals force, the electrostatic force, and magnetic-dipole interactions. If the magnitude of the long-range forces is significant at close tip–surface distances, obtaining atomic resolution can become difficult [1]. Si(111) is the standard surface used in many surface science techniques, including SFM. The complex structure of the 7x7 reconstruction is described by the dimer adatom stacking-faulted model (DAS model) proposed by Takayanagi et *al.* [4]. The uppermost layer consists of six adatoms in each half of the unit cell. These adatoms are bound by covalent bonds formed by $3sp^3$ hybrid orbitals. One of the four $3sp^3$ hybrid orbitals is pointing perpendicular to the surface and forms a dangling bond [5]. Covalent bonding interactions between undercoordinated atoms and unsaturated dangling bonds from the semiconductor surface and the tip are responsible for this atomic resolution [2].

Here, we present the results of our SFM investigations on the Si(111) 7x7 reconstructed surface at RT. We used the FM mode, in which the cantilever is oscillated at its resonance frequency while keeping an oscillation amplitude constant of few nanometers (<10nm). Two feedbak loops keep such magnitudes constant. The signal used to produce the topographic images comes from the forces acting on the tip which are detected as deviations in the cantilever resonant frequency. The typical atomically resolved SFM of Si(111) images show the 12 protruding adatoms and a corner hole for every unit cell. In some cases, also the observance of the restatoms has been reported. However, in our atomic resolved experiments not only the expected images are reproduced, but also several different contrasts are found. The Si(111) surface was crosschecked with STM measurements that proved that the surface was (7x7) reconstructed. For the interpretation of our results, the other parameter images recorded simultaneously, such as the frequency shift, the dissipation, and the current are used for obtaining the correspondence of the structures observed with the DAS model. The different kind of images can be classified as follows:

Normal contrasts:
1- imaging of the adatoms. This is the typical SFM image, similar to STM image for V>0 (empty states) with the 12 adatoms and a corner hole per unit cell, see Figure (a)&(b);
2- imaging of adatoms plus restatoms. This image is also similar to STM image but in this case for V<0 (filled states) with the 12 adatoms plus a weak signal of the 6 restatoms and a corner hole, Figure (c);
3- imaging of the restatoms. The 6 subsurface restatoms and a corner hole are imaged. No signal of the adatoms is measured although they are still there, like they would be transparent, see Figure (d).

Inverted contrasts:
4- complementary image: the “holes” between adatoms are imaged as protrusions. The corner holes look as brigther protrusions, whereas the ones between the restatoms look darker, see Figure (e);
5- complementary image with darker corner holes. In these images the protrusions have all the same appearance but the corner holes look again dark. Different protrusions and corner holes shapes are observed, sometimes circular, sometimes more star-shaped, see Figure (f)&(g);
6- bright corner holes. Again adatoms are resolved as protrusions, but some of them are not visible since the corner holes appear very bright and larger that their original size covering them, see Figure(h).

For the SFM experiments silicon cantilevers were used, some of them were coated with PtIr. Different treatments were applied to the cantilevers: in some cases we dipped them in organic solvents before introducing it into the vacuum chamber. In UHV, the majority of the tips were heated to 140°C, and for some experiments the cantilevers were sputtered in order to remove their native oxide layer. In general, the images were measured with a value of the bias that compensated the contact potential difference between the tip and the semiconductor surface. A switch between some of the contrasts was possible by only changing the frequency shift, i.e., by changing the distance to the surface.

The shape and nature of the tip together with its changes produced during scanning resulted in various kinds of interactions with the semiconductor surface giving rise to different contrasts. These are not only produced by a strange tip, since they have been reproduced with several cantilevers.

References

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Figure

Different contrasts in the FM-AFM images

Normal contrasts: (a)&(b) adatoms; (c) adatoms + restatoms; (d) restatoms.
Inverted contrasts: (e) complementary; (f)&(g) complementary + dark corner holes; (h) bright corner holes. Images size 7 x7 nm^2. DAS model is superimposed on the FM-AFM images.