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Review

What is the orientation of the tip in a scanning tunneling microscope?

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ABSTRACT

The atomic structure and electronic properties of the tip apex can strongly affect the contrast of scanning tunneling microscopy (STM) images. This is a critical issue in STM imaging given the, to date unsolved, experimental limitations in precise control of the tip apex atomic structure. Definition of statistically robust procedures to indirectly obtain information on the tip apex structure is highly desirable as it would open up for more rigorous interpretation and comparison of STM images from different experiments. To this end, here we introduce a statistical correlation analysis method to obtain information on the local geometry and orientation of the tip used in STM experiments based on large scale simulations. The key quantity is the relative brightness correlation of constant-current topographs between experimental and simulated data. This correlation can be analyzed statistically for a large number of modeled tip orientations and geometries. Assuming a stable tip during the STM scans and based on the correlation distribution, it is possible to determine the tip orientations that are most likely present in an STM experiment, and exclude other orientations. This is especially important for substrates such as highly oriented pyrolytic graphite (HOPG) since its STM contrast is strongly tip dependent, which makes interpretation and comparison of STM images very challenging. We illustrate the applicability of our method considering the HOPG surface in combination with tungsten tip models of two different apex geometries and 18,144 different orientations. We calculate constant-current profiles along the $\langle 1\bar{1}00\rangle$ direction of the HOPG(0001) surface in the $|V| \leqslant 1$ V bias voltage range, and compare them with experimental data. We find

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that a blunt tip model provides better correlation with the experiment for a wider range of tip orientations and bias voltages than a sharp tip model. Such a combination of experiments and large scale simulations opens up the way for obtaining more detailed information on the structure of the tip apex and more reliable interpretation of STM data in the view of local tip geometry effects.

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1. Introduction

The interpretation of scanning tunneling microscopy (STM) images is not straightforward due to the effects of the local tip apex geometry, termination and orientation. The reason is the convolution of sample and tip electronic states in a given energy window defined by the bias voltage, and the fact that in STM experiments the detailed atomic geometry around the tip apex is practically unknown and hardly controllable. On the other hand, it is clear that the electronic states and their dominating orbital characters involved in the tunneling depend very much on the local atomic structure of the tip apex.

It has been a challenge to obtain information about the relevant properties of the STM tip apex for a long time. Herz et al. performed reverse STM imaging experiments to study *p*, *d*, and *f* orbital characters of the tip apex atom above the Si(1 1 1)-(7 × 7) surface [1]. The combination of STM experiments and simulations on well characterized surfaces to obtain information on the tip structure and termination was used, e.g., by Chaika et al. [2,3]. They considered the highly oriented pyrolytic graphite (HOPG) surface in the (0 0 0 1) crystallographic orientation in combination with W(0 0 1) tip models. Rodary et al. studied Cr/W tip apex structures by high resolution transmission electron microscopy, and they pointed out that the magnetization direction of monocrystalline nanotips cannot be controlled in spin-polarized STM [4]. Recently, the effect of the tip orbitals on the STM imaging of supported molecular structures attracted considerable attention. Gross et al. investigated pentacene and naphthalocyanine molecules on NaCl/Cu(1 1 1) surface by CO-functionalized tips, and they explained the obtained STM contrast by tunneling through the *p*-states of the CO molecule [5]. Siegert et al. developed a reduced density matrix formalism in combination with Chen's derivative rule [6] to describe electron transport in STM junctions for molecular quantum dots, and studied the effect of selected tip orbital symmetries on the STM images of the hydrogen phthalocyanine molecule on a thin insulating film [7]. Lakin et al. proposed a method to deconvolute STM images and determine molecular orientations of both the sample and the functionalized tip [8]. In their work a C_{60}–Si(1 1 1)-(7 × 7) surface and a C_{60}-functionalized tip were chosen.

Even in seemingly less complicated STM junctions, only a few theoretical works focused on the effect of the tip orientation on the STM images. Hagelaar et al. demonstrated that a wide range of modeled tip terminations and orientations can reproduce the experimental images for NO adsorbed on Rh(1 1 1) [9]. This work also showed that the modeling of realistic tip structures, including nonsymmetric tips, is desirable for a good qualitative reproduction of experimental STM images. However,