Simulation of scanning tunneling microscopy from first principles

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Summary

Since its invetion in the 1980's scanning tunneling microscopy (STM) contributed to the rapid development of nanoscience and nanotechnology, and has been actively used in many subfields of surface science to study a wide spectrum of materials' surfaces.

STM does not image the geometric structure of the surface, but the combination of the atomic geometry and the convolution of electron densities of states of the sample and the tip. This can highly complicate the interpretation of experimental STM images, therefore theoretical modeling of the STM is highly required, which was the main topic of PhD research.

I made essential contributions to the theoretical development and implementation of the orbital-dependent 3D-WKB tunneling model for the simulation of high-resolution STM and SP-STM images. I investigated the corrugation inversion phenomenon depending on the tip-sample distance and bias voltage observed on the nonmagnetic W(110) and on the magnetic Fe(110) surfaces, and explained the phenomena based on the real-space shape of the electron orbitals, and also by the complex interplay of electron densities of states of the sample and the tip.

I extended the model to handle arbitrary tip orientations and studied the W(110) surface with numerous tip orientations, and the complex dependence of the contrast inversion on the tip-sample distance, bias voltage, and tip orientation was uncovered and explained. I also studied the tip-rotational effects on the STM images of the highly oriented pyrolytic graphite (HOPG) surface, and found that $m \neq 0$ tip-apex electronic states can cause a triangular-hexagonal change in the primary contrast.

I introduced a novel correlation analysis method to quantitatively evaluate the degree of agreement between STM images obtained by different theoretical methods or experimental data and also a statistical analysis method to obtain information on the local geometry and orientation of the tip used in STM experiments.

I revised Chen's derivative rule for the purpose of simulations based on first-principles electronic structure data. By applying it to two functionalized surfaces where quantum interference effects play an important role in the STM imaging process (N-doped graphene and a magnetic Mn_2H complex on the Ag(111) surface) I showed that the interference between s and p_z tip orbitals can cause a significant contrast change.

Both introduced methods are proved to be a fast and reliable tool for calculating STM images taking into account the electronic structure and local geometry by arbitrary tip orientations.