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Theoretical study on tunneling current flowing between STM tip and acetylene-adsorbed Si(001) surface

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Abstract

We present first-principles electron-transport studies on scanning tunneling microscopy (STM) images of an acetylene-adsorbed Si(001) surfaces. In the simulated STM images, bright spots are observed in bare Si atoms and darker spots locates on the absorbed acetylene molecule. Tunneling current flowing between the sample and a STM tip is strongly affected by the π states of bare Si atoms and the contributions of states around the molecule to the current are smaller. This causes the STM images where bare Si atoms look higher than the adsorbed molecule.

Introduction

The adsorption of hydrocarbon molecules on a semiconductor surface systems are important for technical applications and have received much attention. In this decade, the adsorption configurations of acetylene (C_2H_2) molecules on the Si(001) (C_2H_2/Si(001)) surface have been experimentally investigated using the scanning tunneling microscope (STM) and several different adsorption configurations are found. However, some of these studies reported that observed STM images are in disagreement with the actual atomic configurations, namely, the bright spots are observed in bare Si atoms which are geometrically lower than C_2H_2 molecules[1)].

In this study, we perform the first-principles calculation for the tunneling current flowing between a tip and samples in order to provide a more profound understanding for the generated STM images for C_2H_2/Si(001) surfaces.

Computational Scheme

Our computational scheme is based on real-space finite-difference approach within the framework of density functional theory[2)]. The norm-conserving pseudopotential and the local density approximation are employed. The electron conduction properties of the

nanostructure are examined using the overbridging boundary-matching method[2]. Here, we adopted two types of di-σ bonding configurations (on-top and end-bridge di-σ configurations).

Results and Discussions

The simulated STM images with a sample bias of -1.5 V is shown in Fig. 1. In the images, there are dark spots on the C_2H_2 molecules and bright spots on the bare Si atoms. This is in agreement with the experimental results. Furthermore, the scanning tunneling spectra, energy band structures and channel current distributions are investigated. From the results, we found thath the π state of the bare Si atom with large contributions to the tunneling current is passivated by the adsorption of the C_2H_2 molecule, and the contributions of the states around the molecule are smaller than those around bare Si atoms. Therefore, the dark spots are observed on the molecule.

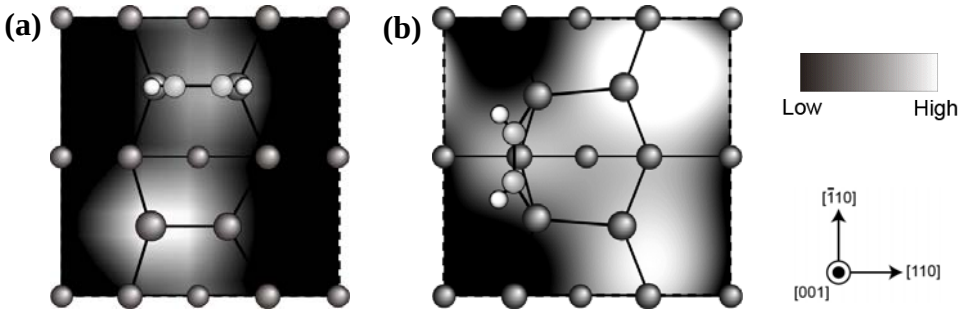

Fig. 1. Calculated STM images for (a) on-top di-σ and, (b) end-bridge di-σ configurations. Dark gray, light gray and white spheres represent Si, C and H atoms, respectively.

Conclusions

We performed first-principles calculations for the tunneling current flowing between the C_2H_2-adsorbed Si(001) surface and the tip to investigate the experimental STM images of the C_2H_2/Si(001) system. In the resultant STM image, when the STM tip locates above the C_2H_2 molecule, the tunneling current decreases compared with that in the case of the tip locating above the bare Si atom owing to small contributions of states around the molecule to the tunneling current. Eventually, the absorbed C_2H_2 molecules geometrically look lower than bare Si atoms in the STM images.

References

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