STM/STS investigation of silicon adatoms

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Scanning Tunneling Microscopy (STM) and Scanning Tunneling Spectroscopy (STS) are two complementary techniques capable of resolving structures and studying electronic transport on atomic scale. In this letter we report on topographic characterization of boron passivated Si(111) surface and on electronic transport measurements performed on passivated and unpassivated silicon adatoms. The topographic measurements revealed the presence of unpassivated silicon dangling bonds (DB) on B/Si(111) $\sqrt{3}\times\sqrt{3}$ R30° surface whilst the spectroscopic measurements revealed the electronic structure of the two types of silicon adatoms: passivated and unpassivated ones. The presence of a dangling bond state inside the band gap, completely decoupled from any other state, is used to explain the topographical contrast observed in STM images and the high tunneling currents measured in STS experiments.

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1. Introduction

In the recent years Scanning Tunneling Microscope (STM) has become the most ubiquitous tool in surface science capable of imaging, fabrication or characterization of nanoscale structures. It is well known that STM is able to image and resolve orbitals of single molecules and charge states of single atoms [1]. Using Scanning Tunneling Spectroscopy (STS) as a complementary technique the study of electronic transport on atomic scale can be achieved.

Electronic transport through atomic systems is a very hot research topic with important consequences for the development of new research fields such as molecular electronics [2]. On the other hand silicon is a material of extreme importance in semiconductor technology and its surface was one of the first materials investigated by STM [3].

In this letter we report on topographic and electronic transport measurements performed on silicon passivated adatoms and localized unpassivated silicon dangling bond states which can be considered single quantum levels. By using the STM tip as an electrode and a B-passivated Si(111) $\sqrt{3}\times\sqrt{3}$ R30° surface as another electrode the conductance of an unpassivated Si adatom was measured. The electronic structure of this adatom corresponds to a dangling bond (DB) state localized in the silicon band gap and completely decoupled from any other state. The topographic measurements revealed the presence of Si adatoms dangling bonds (DB) on B/Si(111) $\sqrt{3}\times\sqrt{3}$ R30° surface whilst the spectroscopic measurements performed on these dangling bonds indicated the existence of an unusually high tunneling current.

2. Experimental details

The experiments have been carried out by using a low temperature, ultra high vacuum Omicron Scanning Tunneling Microscope (Omicron UHV LT STM) having a base pressure of $2x10^{-10}$ Torr on a boron doped Si(111) surface. The boron doped silicon surface has been prepared at temperatures higher than 900 °C in ultra high vacuum conditions (UHV). The sample was degassed overnight at a temperature of 950°C with a base pressure of $5x10^{-10}$ Torr and than the temperature was decreased at ~900 °C and kept at this value in order to allow the segregation of boron dopants to the surface.

The topographic images have been achieved using a voltage bias between -2V and +2V and a feedback current between 100pA and 1nA while the spectroscopic measurements have been taken for bias voltages in the range -2V, + 2.5V and feedback currents between a few hundreds of pA to a few nA. In order to reduce the influence of the transmission coefficient and to diminish the background noise a large number of spectra (more than 100 for each spectroscopic measurement) has been taken and averaged. The spectra displayed in this paper amount to the differential conductivity (dI/dV) or normalized differential conductivity $(dI/dV)(I/V)^{-1}$ vs. Bias Voltage for different regions of the silicon surface.

3. Results and discussion

As a result of thermal treatment, the boron atoms segregate through the surface and substitute most of Si atoms located just under the Si adatom position, causing the passivation of the adatom dangling-bond (DB) states by a charge transfer process from the Si adatom to the substitutional B [4]. For a few minority sites, the substitution does not take place, leaving their dangling bond states unpassivated and localized in the band gap region of silicon.

In Fig. 1 a constant-current STM image of a B-doped Si(111) surface acquired at 77 K is shown. Due to the positive polarization of the surface (+2V) with respect to the tip, the electrons will flow from the tip to the unoccupied states of the surface. For this reason the image will be called an empty states STM image.

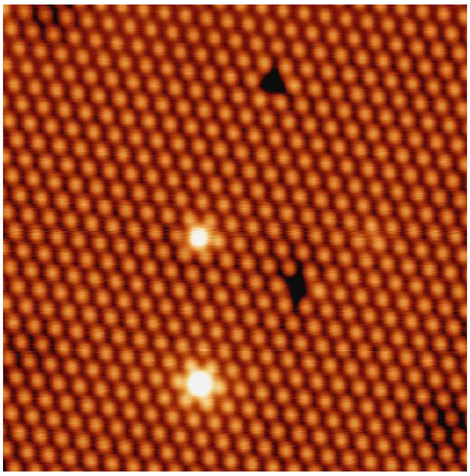

Fig 1. Visualization of passivated and isolated Si dangling bonds on the B/Si(111) $\sqrt{3}\times\sqrt{3}$ surface observed at 77 K. The majority of the adatoms appears dark (adatoms with B atoms underneath). Unlike these adatoms, two Si adatoms appear much brighter and correspond to a configuration with a Si atom underneath (unpassivated Si dangling bonds). Two missing adatoms can also be observed (black depressions). The image was taken at V_{sample}=+2V (empty state STM image).

As it can be seen on the image, most of the Si adatoms appear dark, consistent with the passivation of the DB states. However, two isolated bright adatoms can be seen. Their corresponding DB wave functions are localized into the region defined by the six first surface neighbors of the adatom, giving rise to a bright flowerlike shape. Two missing silicon adatoms can also be observed on the surface (black depressions).

The same region has been topographically imaged at a negative bias (V_{bias}=-0.8V). In this case the electrons will flow from the surface to the tip and the resulting topographic image will be called filled state STM image (Fig. 2).

The numerous bright protrusions, which show a more or less dark contrast in the empty state image, correspond to subsurface B dopants, located at least 4 atomic layers below the surface [5]. The boron dopants create an acceptor band very close to the valence band (p-type semiconductor) and at low negative bias these states are visible in the filled state STM image. It has to be noticed that the faint dark depressions observed in fig.1 turn into protrusions when chainging the voltage sign to image filled states (Fig. 2). These features are the signature of subsurface dopant atoms. They result from the local screened Coulomb potential-induced band bending surrounding the charged B impurities [5,6].

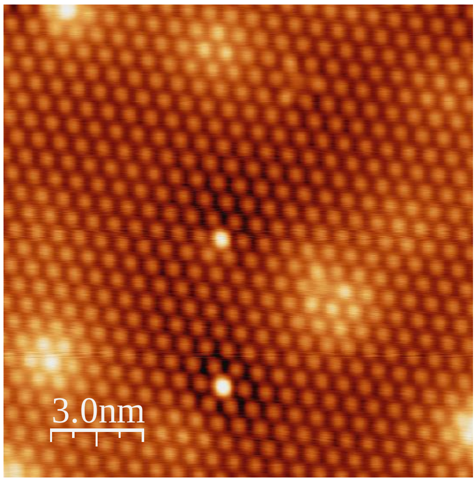

Fig. 2. Filled state STM image of the area plotted in figure 1 (V_{bias}=-0.8V). The bright protrusions correspond to boron dopants located at least 4 atomic layers below the surface. The areas of the two scanned regions plotted in Figs.1 and 2 are the same: 15x15 nm^2.

In order to establish a direct link between the topographic images and their electronic nature, scanning tunneling spectroscopy (STS) measurements have been performed on the two types of adatoms: bright adatoms, corresponding to unpassivated dangling bonds, and dark adatoms (corresponding to boron passivated dangling bonds).

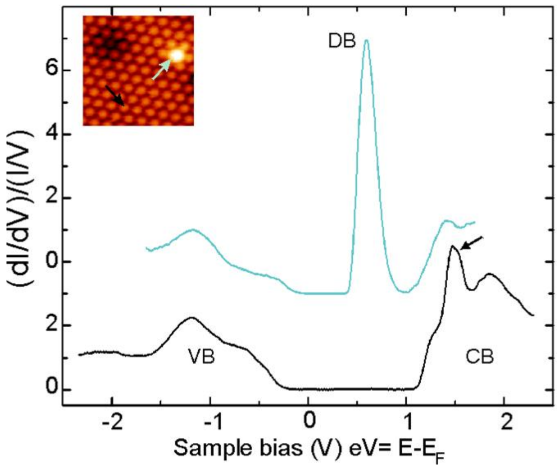

Fig. 3. Normalized conductivity spectra of passivated (black curve) and unpassivated (blue curve) silicon adatoms. The inset shows a topographical image of the two adatoms (bright and dark) where the spectroscopic measurements were acquired. The topographic image was taken at V_{bias}=+2V, corresponding to an STM empty state image. The strong peak associated with the unpassivated dangling bond (DB) is localized inside the semiconducting band gap (blue curve). The valence band and the conduction band of passivated silicon are labeled with VB and CB, respectively.

As it can be seen in Fig. 3 the spectrum acquired on a Si passivated adatom (black curve) has the typical shape of a p-type semiconductor: the Fermi level E_F is positioned very close to the valence band (VB) due to the acceptor band formation by boron doping and a well defined band gap of about 1.3 eV can be observed. In contrast with this typical spectrum, when the spectroscopic measurements were performed on unpassivated Si dangling bonds an unusual feature can be observed in the band gap (blue spectrum). A distinct peak centered at an energy of ~0.65 eV is visible in the band gap. It is associated with a nonresonant dangling bond state of the unpassivated adatom. The presence of this peak explains the strong topographical contrast of the two types of silicon adatoms in the empty state image (Fig. 1) [7]. Surprisingly these unpassivated dangling bonds can hold currents higher than 10 nA at 5K even if they are completely decoupled from any other state. Recent studies performed on this system showed that the electronic transport is assisted by local polarons at the interface atoms [7,8].

4. Conclusions

In summary, with the aid of a scanning tunneling microscope (STM) operating at low temperatures the topographic images of the boron doped Si(111) $\sqrt{3}\times\sqrt{3}$ R30° surface in the empty state and the field states were taken. Secondly, by using the STM tip as one electrode and the passivated surface as another, scanning tunneling spectroscopy measurements have been performed on both types of adatoms: passivated and unpassivated ones.

The electronic structure of the passiveted adatoms is typical for a p-type semiconductor having the Fermi level very close to the valence band. The presence of an acceptor band in the proximity of the Fermi level explains the topographical images obtained in the filled regime where the subsurface boron dopants located under the surface are visible.

In the case of unpassivated adatoms, the electronic structure of this adatom corresponds to a DB state energetically localized in the energy gap of the surface. Hence, this state is electronically decoupled from any other electronic state. The presence of this state inside the band gap explains the strong topographical contrast of the two types of silicon adatoms in the empty state STM image. Surprisingly these decoupled quantum levels can support currents higher than 10 nA.

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