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A parabolic quantum well on a single dimer row of the Si(001) surface studied by scanning tunneling spectroscopy

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Abstract. Quantum confinement in a single silicon dimer row of the Si(001) surface is presented with data obtained by scanning tunneling spectroscopy. The structure to confine surface electrons was made by depositing tungsten atoms on a silicon dimer row from the tip. The tungsten atoms not only scattered electrons, but also modified potential features of silicon dimers close to them, resulting in the reduction of the effective width of the quantum well. Confinement in this structure is, therefore, explained by a parabolic potential well.

1. Introduction

Quantum confinement offers an opportunity for seeing how an electronic structure in a system is modified by decreases in dimension. For surface states, confinement has been studied by taking advantage of the unique ability of scanning tunneling microscopy (STM) and spectroscopy (STS) to manipulate atoms and to probe electronic states [1–8]. Most experiments, thus far, were performed on noble metal surfaces. However, a study on semiconductors would provide a more practical understanding of optical and memory device applications. For this purpose, the Si(001) surface is a good candidate for studying quantum phenomena since Si(001) exhibits the quantum interference of surface state electrons [9, 10].

The dimer row of the reconstructed Si(001) surface possesses unique surface electronic properties originating from the dangling bonds. The empty dangling bond (π^*) state is situated within the bulk band gap and reveals energy dispersion only along the dimer row, while the filled dangling bond (π) state is overlapped by the bulk valance band [11, 12]. Hence, the π^* band exhibits quasi one dimensional (1D) characteristics, which have been confirmed by observations of surface standing waves using STM [9, 10].

Previously, we reported fabrication of a quantum well (QW) on a single Si dimer row by depositing tungsten (W) atoms from the STM tip [13]. Deposited W atoms acted as potential barriers scattering electrons injected to the π^* state. Here, we revisited the same system to model quantum confinement in a single dimer row and to extract the effective mass of the π^* state.

2. Experiment

Experiments were performed on an ultrahigh vacuum - low temperature STM (Unisoku USM-1200). The sample we used was an n-type Si wafer with resistivity of 0.003 Ωcm. To obtain a clean surface, a piece of Si wafer was flashed to 1200 K in a base pressure of 3×10^{-9} Pa. Afterwards, the sample was cooled to 79 K. STM imaging and STS measurement were done with an electrochemically etched tungsten tip. The differential conductance (dI/dV) maps and tunneling spectra were acquired through a lock-in amplifier using a voltage modulation (20 mV, 6.5 kHz).

3. Results and Discussion

The top image in Figure 1 shows a constant current image of the QW made on a single Si dimer row. The protrusions separated by 9.2 nm were W atoms deposited from the STM tip by using the tip-sample point contact technique. The detailed procedure to make this structure is described in ref [13]. One dot of W atoms appears to consist of two W atoms, so hereafter we will call it a W dimer. The W dimer acted as a potential barrier to scatter incoming electron waves along the relevant Si dimer row. Since the motion of electrons in the empty π^* state is limited within a single Si dimer row with its electronic property [9–12], electrons were confined in a 1D potential well consisting of the section of the dimer row that is between two W dimers.

The other images in Figure 1 show the dI/dV maps recorded in the same area for different sample biases. As the sample bias was raised, the number of confined states evolved from n=1 to n=5. The W dimers also exhibited strong dI/dV signals at the center of each dimer in the sample bias range between +0.22 V and +0.52 V, while the signal was localized above the W atoms below +0.20 V. The enhanced conductance between W atoms indicates strong coupling between W atoms [6].

Moreover, we observed that the effective width of the potential well was decreased with a smaller sample bias. This indicates that the cross section of the 1D potential well that was made by the W atoms deposition was not square, but rather of a slowly-varying-in-space shape. Obviously, the adsorbed W atoms modified the potential of the Si dimers close to them. Their influence was greater at a smaller sample bias and extended to at least the sixth Si dimer away from the W atoms at

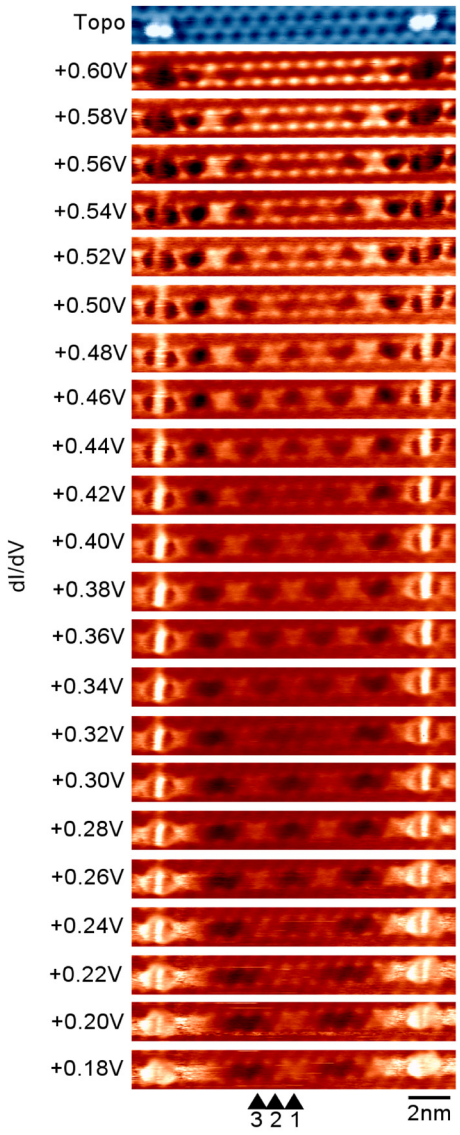

Figure 1. Constant current image (topography) of the quantum well made on a single Si(001) dimer row (top image) and differential conductance (dI/dV) images for different sample biases (others). The bright protrusions are tungsten atoms deposited from the STM tip.

a sample bias of +0.20V. If the W dimers bore an excess charge, they should have modified potential energy around them by the screening effect. In fact, a dopant atom (phosphorous) with an excess charge in the topmost Si(001) surface has been observed to cause band bending on Si dimers around it [14]. However, the modification in the potential shape occurred only along the dimer row adsorbed by the W dimers, which was confirmed by the fact that standing waves were not formed in the neighboring Si dimer rows. Hence, the slowly-varying-potential was realized rather by stress or some other effect through the W atom adsorption.

We attempted to theoretically relate wave functions to the result in Figure 1, which requires knowing the shape of a potential well. Determination of the shape of the potential well would demand more detailed STS experiments around the W dimers or perhaps theoretical supports. However, we can approach this problem in a different way. The tunneling spectra measured at the three locations within the QW and at a Si dimer outside of the QW are presented in Figure 2. Differing from the spectrum on a Si dimer outside of the QW, the spectra in the QW showed oscillating features with five bound states, which is consistent with the results in Figure 1. Also, we found that the energy levels for each quantum state are equally spaced. This allows us to deduce that surface electrons were trapped in a parabolic well. Energy levels for a parabolic well are given by [15]:

$$E_n = \left(n - \frac{1}{2}\right)\hbar\omega_0, \quad n = 1, 2, 3, \ldots \tag{1}$$

where ω_0 is angular frequency and $\hbar = h/2$ (h: Planck's constant). The energy separation $\hbar\omega_0$ for our QW was determined from Figure 2 to be approximately 79 meV. Accordingly, we employ the wave functions in the parabolic well, which are described using Hermite polynomials H_n as [15]:

$$\phi_{n+1}(x) = \left(\frac{1}{2^n n!\sqrt{\pi}}\right)^{1/2} \left(\frac{m_0 m^* \omega_0}{\hbar}\right)^{1/4} exp\left(-\frac{m_0 m^* \omega_0 x^2}{2\hbar}\right) H_n\left[\left(\frac{m_0 m^* \omega_0}{\hbar}\right)^{1/2} x\right] \tag{2}$$

where m_0 is the mass of the free electron. To fit this equation to the experiment data, the only parameter that we need to determine is the effective mass m^* of the π^* state. Figure 3 displays the cross sections of the selected dI/dV maps fitted by the squared wave functions for the parabolic well. The dI/dV maps were chosen from Figure 1 at the sample bias where the oscillating tunneling spectra in Figure 2 exhibited the local maximal value. Fitting by the squared wave functions for the parabolic well agreed with experimental data. The value for m* in the dimer row direction that we obtained is 0.52 ± 0.056, which is almost as twice as large as that reported previously [9]. This discrepancy may be attributed to determination of the effective width of the QW. In our case, the effective width (e.g. 4.0 nm for $n = 1$ and 7.7 nm for $n = 5$) is smaller than the measured width (9.2 nm). In ref. [9], the authors, in contrast, used constant current imaging to probe the QW on Si(001), which was modeled with a square potential well. In their analysis, the accuracy required to extract the effective mass was affected by the width of the QW. However, the constant current images are apt to overestimate the width of a potential well.

4. Conclusion

We presented quantum confinement in a single Si dimer row sectioned by two W dimers that were separated by 9.2 nm. The W dimer revealed enhanced conductance in the middle of it, which implies that strong coupling occurs between W atoms. Also, the W dimers modified the potential of the Si dimer row near them, resulting in reduction of the effective width of the potential well. Confinement in this structure was thoroughly explained by using a parabolic potential well model. Theoretical fitting using squared wave functions for the parabolic well agreed with the experimental data.

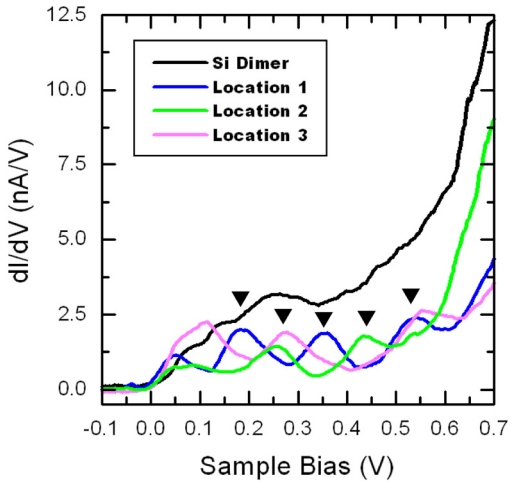

Figure 2. Tunneling spectra from three locations within the QW (indicated by triangles in Figure 1) and a Si dimer outside of the QW.

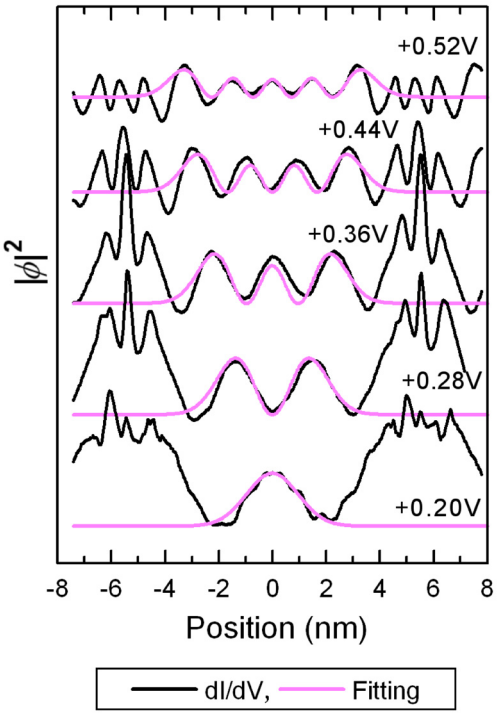

Figure 3. Cross sections of the dI/dV images in Figure 1 for five bound states and fitting curves obtained with a parabolic quantum well model. The effective mass of the Si dimer row used in fitting was 0.52.

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