Probing negative differential resistance on Si(111)-√3×√3-Ag surface with scanning tunneling microscopy

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We present our study on the Si(111)-√3×√3-Ag surface using scanning tunneling microscopy/spectroscopy. The results reveal that the well defined localized surface-state bands $S_2/S_3$ in the surface with lightly doped Si substrate play an important role in electron transport. The relative wide space charge layer beneath the surface interplays with the localized surface states, thus leading to the effect of the negative differential resistance. © 2009 American Institute of Physics.

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Si(111)-√3×√3-Ag surface is a widely studied system\textsuperscript{1} that possesses well-defined surface-state (SS) bands.\textsuperscript{2–8} It is interesting to make use of such SS bands in extension of silicon and silicon-based devices, which may be applied to build circuits based on the concept of hybrid functions.\textsuperscript{9} Our experiments were conducted using an Omicron ultrahigh vacuum low temperature scanning tunneling microscope (STM). A lightly doped n-type Si(111) wafer (P doped with concentration of $5 \times 10^{14}$ cm$^{-3}$) was used. Clean Si(111)-7×7 surface was prepared by degassing Si at 873 K for about 10 h, then flashing to 1500 K for several times, rapidly cooling down to 1200 K and slowly cooling down to room temperature. The Si(111)-√3×√3-Ag surface was obtained by evaporating 1 ML Ag onto the Si(111)-7×7 surface at about 650 K and annealing at the same temperature for 20 min. The sample is referred as Ag/Si−l. For comparison, a heavily doped n-type Si(111) wafer (P doped with concentration of $1 \times 10^{18}$ cm$^{-3}$) was also used (referred as Ag/Si−h). The samples were transferred into the cryostat of the STM in a chamber with a base pressure of $3 \times 10^{-11}$ Torr. The presented data were acquired at 5 K. Tungsten tips were used, which had been subject to careful cleaning treatments.

Figure 1(a) shows the STM image of the Si(111)-√3×√3-Ag surface. The IET structural model\textsuperscript{11,14} is superposed within a unit cell. The two protrusions in different brightness correspond to the two inequivalent Ag triangles in each unit cell, which are denoted as A and B, respectively. The hole at the vertex of the unit cell is denoted as C. Interestingly, as shown in Fig. 1(b), the I-V curves acquired at both sites A and B exhibit NDR at around $-3$ V in Ag/Si−l. There is no NDR in the I-V curve at site C, instead, only a shoulder at around $-3$ V. The results are independent on the different STM tip used. One may note that the slope of the I-V curves is nonzero around $E_F$ [upper in Fig. 1(b)], reflecting its non-zero local density of states (LDOS) [lower in Fig. 1(b)]. The nonzero LDOS at around $-0.3$ V was observed before, and...
is attributed to the contribution of the SS band $S_1$.\cite{11,13,16} Since it is a dispersive, two-dimensional free-electronlike surface state, and far higher than the observed NDR position of $-3 \text{ V}$, the SS band $S_1$ should not contribute to the NDR effect.

As a comparison, a Si(111)-$\sqrt{3} \times \sqrt{3}$-Ag surface was measured in Ag/Si–h, as shown in the inset of Fig. 1(b). In contrast to the NDR feature in Ag/Si–l, only the shoulder feature is observed at all of the corresponding sites in Ag/Si–h. Meanwhile, the position of the shoulder fixes at around $-1 \text{ V}$, independent on the bias and the setpoint conditions. Similar behaviors have been reported in the Si(111)-$\sqrt{3} \times \sqrt{3}$-Ag surface with similarly heavily doped Si wafers, and such shoulder feature at $-1.1 \text{ V}$ in $I$-$V$ curves has been well attributed to the contribution of the SS bands $S_2/S_3$.\cite{11,13,17}

It is noted that NDR only appears in Ag/Si–l, but not in Ag/Si–h. This phenomenon suggests that the existence of the localized SS bands $S_2/S_3$ is a necessary condition, but it is not sufficient. As shown in Fig. 1(c), by sweeping voltage forward (from negative bias to positive bias) and backward (from positive bias to negative bias), although the NDR position does not change, there exists obvious hysteresis between the $I$-$V$ curves in Ag/Si–l, in contrast to the behavior without hysteresis in Ag/Si–h [inset in Fig. 1(c)]. The hysteresis in Ag/Si–l reflects the charging process during electron transport. As we will discuss below, the main factor affecting the $I$-$V$ features in the two samples is the difference in SCL width.

The SCL width can be estimated by $w = [2\varepsilon_e \Phi/(N\varepsilon_0)]^{1/2}$, where $\varepsilon_e = 11.9\varepsilon_0$ is the silicon dielectric constant, $\varepsilon_0$ is the dielectric constant of vacuum, $\Phi$ is the barrier height, and $N$ is the doping concentration.\cite{18} Because the doping concentration in Ag/Si–l is about four orders of magnitude smaller than that in Ag/Si–h, the SCL width in Ag/Si–l is thus larger by about two orders of magnitude than that in Ag/Si–h. As a result, the electron transport between the bulk states and the surface states in Ag/Si–l is much more limited than that in Ag/Si–h. The effect of the SCL in Ag/Si–l is schematically depicted in Figs. 2(a) and 2(b). Before an external bias is applied [Fig. 2(a)], $E_F$ is pinned around the maximum of the valence-band by $S_1$, so that the bulk bands bend upwards in the SCL beneath the surface.\cite{12,13} Under an applied bias, the $E_F$ of the STM tip may only sweep the $S_2/S_3$ bands at a relatively high bias since a fraction of voltage drops at the SCL [Fig. 2(b)]. Thus, the actual voltage for the $E_F$ of the tip matching the bands $S_2/S_3$ should depend on the ratio of the voltage drops between the vacuum gap and the SCL, $V_{\text{gap}}$ and $V_{\text{SCL}}$, respectively.

Such ratio dependent behavior has been confirmed in our experiment. As shown in Fig. 2(c), when the voltage drop at the vacuum gap is increased through increasing the distance of the vacuum gap (decreasing the setpoint current from 140 to 80 pA while keeping bias voltage at $-4.0 \text{ V}$), thus increasing the ratio of $V_{\text{gap}}/V_{\text{SCL}}$, the NDR position systematically shifts toward the $E_F$. Therefore, the large voltage drop at the SCL is a main factor to shift the NDR position in Ag/Si–l, different from the behavior because of small voltage drop at the SCL in Ag/Si–h. Hence, the NDR is originated from the SS bands $S_2/S_3$ in Ag/Si–l, while the NDR position deviated from the energy of the bands is dependent on the ratio of $V_{\text{gap}}/V_{\text{SCL}}$. Moreover, our observations are coincident with the nature of the localized surface states. That is, the bands $S_2/S_3$, consisting mainly Ag 5s and 5p orbitals, are strongly localized at Ag triangles, i.e., at sites A and B.\cite{4,5,14}

Considering the relatively wide SCL in Ag/Si–l, one may expect that the localized surface states are charged due to the low tunneling rate between the Si bulk valence-band states and the surface states. In this situation, when the $E_F$ of the tip matches the SS bands $S_2/S_3$ in $I$-$V$ curve acquisition, say, at $-3.0 \text{ V}$ [Fig. 1(c)], the resonant tunneling occurs. Simultaneously, the wide SCL becomes a dominant constraint, which limits the electron transport and causes a current saturation, thus leading to NDR phenomenon. This process is similar to the NDR behavior due to current saturation in Ref. 19. Generally, since the tungsten is a wide band material, the resonant tunneling between the tip and the surface may not be sufficient to cause NDR,\cite{20,21} which may explain no NDR occurrence in Ag/Si–h.

As shown in Fig. 3, the limited electron transport between the bulk states and the surface states has been observed in the $G$-$z$ curves, i.e., the conductance against the
vacuum gap width. The conductance is numerically obtained by \( G = I / V_f \), where \( I \) is the currents measured in \( I-V \) curves with a fixed bias \( V_f \) in the process of pushing the tip to the surface. With the tip closing to the surface, the conductance increases exponentially at first (dashed line in Fig. 3), followed by a much faster increasing at site A and B (indicated by the arrow), and then becomes almost saturated. The saturated conductance is about 67 pS, which is nearly independent on the bias voltages (inset in Fig. 3). Such behavior in the \( G-V \) curves is also understandable according to the ratio of the voltage drops between the vacuum gap and the SCL. When the tip is far from the surface, the applied bias mainly drops at the vacuum gap, making the \( E_F \) of the tip below the bands \( S_2/S_3 \). In this regime, the vacuum gap is dominant, and the current, thus the conductance, exponentially increases with the decrease of the gap width. Until the \( E_F \) of the tip matches the bands \( S_2 \), the resonant tunneling reaches, corresponding to the faster increasing conductance. This phenomenon is only observed at sites A and B, which is consistent with our discussion above that the localized surface states at sites A and B play a key contribution to the NDR. With the tip further closing to the surface, the SCL becomes dominant since the tunneling rate between the surface and the tip becomes larger than that between the surface and the Si bulk. In this latter regime, the electron transport is limited by the SCL because of its extremely low carrier concentration, leading to the conductance saturation. The nearly unchanged saturation value of 67 pS at different biases mainly reflects the conductance of the SCL [inset in Fig. 3]. In contrast, no such saturated conductance has been observed in Ag/Si−h, because the SCL dominant situation is difficult to be reached due to the relatively high conductance of the narrow SCL in Ag/Si−h.

In conclusion, we have studied the electron transport of Si(111)−\( \sqrt{3} \times \sqrt{3} \)-Ag surface by comparing the results obtained with lightly and heavily doped Si substrates. We find that the well defined localized SS bands \( S_2/S_3 \) may produce NDR in the case of lightly doped Si substrate, where the wide SCL beneath the surface interplays with the localized surface states. Such behavior may be useful in design of hybrid devices.

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