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Electronic structure of Ag-induced atomic wires on Si(5 5 7) investigated by STS and angle-resolved photoemission

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ABSTRACT

One-dimensional (1D) superstructures on the Si(5 5 7) surface induced by Ag adsorption have been investigated by scanning tunneling microscopy/spectroscopy (STM/STS) and angle-resolved photoemission. The deposition of ~0.3 ML of Ag at 450–620 °C yields three different kinds of 1D structures along step edges. These structures form domains of different morphology, whose areal ratio depends on the growth temperature. They commonly share a characteristic atomic-scale wire structure with a ×2 periodicity. These structures are insulating with a band gap of about 0.5 eV as revealed by STS and confirmed consistently by angle-resolved photoemission, in clear contrast to the very recent inverse photoemission result (Phys. Rev. B 77 (2008) 125419).

1. Introduction

Atomic-scale wires created on semiconductor surfaces have attracted great interests because of their potential to be the basis for nanoscale devices and of exotic one-dimensional (1D) physics, such as density-wave formation and non-Fermi liquid behaviors [1–3]. A well-known example is the Si(1 1 1)-4 × 1-In 1D metallic system, which exhibits a phase transition into a 8 × 2 phase at low temperature [1]. The transition was found to be of a metal-insulator type accompanying a charge–density–wave (CDW) formation. Novel dynamics through the CDW formation [4,5] and soliton excitations [6] were observed with atomic resolution by means of scanning tunneling microscopy (STM).

More recent efforts to create such atomic-scale wires have utilized highly vicinal substrates. These substrates act as good templates to grow various 1D structures because of their intrinsic anisotropy; regular arrays of straight steps and narrow terraces [7]. One widely used vicinal silicon substrate is Si(5 5 7) which is miscut from (1 1 1) by 9.5° [8]. The deposition of Au and Pb followed by annealings induces well-ordered atomic-scale wire arrays [7,9,10]. A Peierls-type metal-insulator transition and a unique conductivity transition from 2D semiconducting to 1D metallic conduction were reported on Au/Si(5 5 7) and Pb/Si(5 5 7), respectively [11,12].

Fabricating atomic wires with different metals on this substrate would be interesting for exploring different aspects of 1D metals. However, in contrast to the Au and Pb cases, there have been very few studies on the adsorption of the other metals to date [13,14]. However, very recently, an interesting report was made on Ag/Si(5 5 7), which claimed the observation of a partly ordered 1D structure by STM. Moreover the 1D metallic property and its similarity to the Au/Si(5 5 7) surface were claimed [15].

Motivated partly by this report, we have performed an STM and angle-resoved photoemission (ARP) study on Ag/Si(5 5 7) to detail its structures and electronic band structures. Unlike the Au case, Ag does not largely change the initial morphology of the bare Si(5 5 7) substrate with regularly bunched steps [16] on most of the surface areas although minor domains of (5 5 7) and (4 4 5) facets are also formed depending on the growth temperature. The three different domains commonly have an atomic wire structure with a $2a_0$ periodicity along the wires (a_0 = 0.384 nm, the lattice constant of Si(1 1 1)) in accord with the previous STM study [15]. However, these wires are clearly insulating with a large band gap in scanning tunneling spectroscopy (STS). The ARP measurement confirms that the surface as a whole is insulating with only dispersionless surface states at 0.7 and 1.2 eV below the Fermi level (E_F). This contradicts with the claim of the inverse photoemission study [15]. The present results are discussed in comparison with different Ag- and Au-induced phases on vicinal Si substrates.

2. Experimental

The experiments were performed in two separate ultrahigh vacuum systems with base pressures better than 1×10^{-10} torr. The ARP measurements were performed using a high-resolution electron analyzer (SES-100, Gammadata, Sweden) and the He I radiation ($h\nu$ = 21.2 eV). The instrumental angular and energy

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resolution is set better than 0.15° and 20 meV. STM images were obtained by a commercial microscope (Omicron, Germany). All measurements were performed at room temperature. A clean Si(5 5 7) surface was obtained by heating with a direct current flow through the sample up to 1250 °C shortly followed by a careful quenching and annealing procedure [8]. This yielded a low-energy electron diffraction (LEED) pattern of Fig. 1a, which consists of rows of spots along the [7 7 $\bar{1}$0] direction repeating with the ×7 periodicity in the [1$\bar{1}$0] direction. This is consistent with the previous studies [10,17] and evidences the characteristic triple-step structure, which is composed of alternating (1 1 1) and (1 1 2) facets as referred to the 'hill-and-valley' unit [8]. The (1 1 1) facet is covered with the 7 × 7 structure which yields the ×7 features in LEED. Ag was evaporated from a well outgassed graphite effusion cell onto this substrate held at various temperatures from room temperature up to 700 °C. The Ag coverage (Θ_{Ag}) was estimated by referring to the Si(1 1 1)–$\sqrt{3}$ × $\sqrt{3}$–Ag surface at Θ_{Ag} = 1.0 ML.

3. Results and discussion

Fig. 1b displays the LEED pattern after the deposition of 0.4 ML Ag at 500 °C. Streaky spot arrays along [7 7 $\bar{1}$0] and faint ×2 streaks between them are observed as reported previously [15]. This pattern develops above 450 °C. This streaky pattern evolves into a more well-defined spot array above 550 °C (Fig. 1c), where the periodicity along [7 7 $\bar{1}$0] can reliably be measured as ×8.7 (3.34 nm). Beyond 620 °C, the desorption of Ag occurs and the LEED pattern gradually changes into that of the bare Si(5 5 7) surface. These more or less ordered 1D features in LEED are observed at the Ag coverage of 0.2 < Θ_{Ag} < 0.4 ML. They indicate the formation of a partly ordered 1D structure with some ×2 modulation along [1$\bar{1}$0] by Ag adsorption after removing the 7 × 7 reconstruction. No ordered feature is found below Θ_{Ag} = 0.2 ML and the LEED pattern for the Si(1 1 1)-$\sqrt{3}$ × $\sqrt{3}$-Ag surface appears above Θ_{Ag} = 0.4 ML, in the above temperature range. The latter indicates that the regular step array becomes unstable against an active step bunching to yield wide (1 1 1) terraces.

In order to characterize this 1D structure further, we have performed an STM investigation. Fig. 2a shows an empty-state STM image of the Ag/Si(5 5 7) surface formed at 590 °C. The surface is covered mainly with largely corrugated units. The corrugation is very similar to those on bare Si(5 5 7) as compared in the inset of

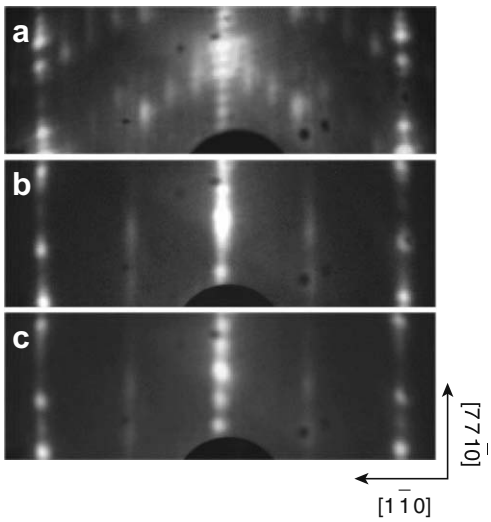

Fig. 1. LEED patterns of (a) the clean surface and (b) and (c) the Ag-induced ×2-structured surface on Si(5 5 7). The sample was prepared at 500 and 610 °C during Ag deposition on (b) and (c), respectively. The incident electron energy was 40 eV.

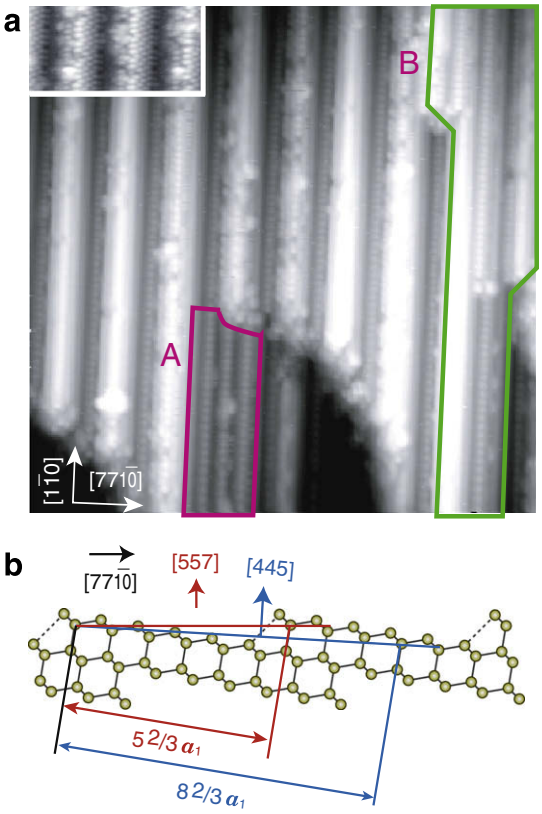

Fig. 2. (a) An empty state STM image of the Ag/Si(5 5 7) surface annealed at 590 °C (50 × 50 nm^2). The sample bias (V_s) and the tunneling current (I_t) were V_s = 1.0 V and I_t = 2 pA, respectively. The surface is covered mainly with the hill-and-valley domain, and partly with the truncated (5 5 7) and the (4 4 5) domains labeled as *A* and *B*, respectively. An STM image of the bare Si(5 5 7) surface (V_s = 1.0 V and I_t = 10 pA) is shown in the inset. (b) A ball and stick model of a truncated Si(5 5 7) surface.

Fig. 2a, whose unit cell has a width of 17a_1 (where $a_1 = a_0 \cos 30°$). That is, the basic hill-and-valley morphology of the substrate seems not to be significantly modified by Ag deposition in clear contrast to the cases of Au (Ref. [11].) and Pb [12]. In those cases, the triply bunched steps are debunched to form uniform (5 5 7) or (2 2 3) facets with single steps, respectively. However, the 7 × 7 reconstruction is completely removed indicating that the atomic structure of the surface is largely affected by the Ag adsorption. The atomic scale features after the Ag deposition is not so easily resolved in STM, especially on the hill part of the corrugation with various irregular protrusions. On the other hand, in the valley part, very well ordered rows of bright protrusions are observed with a well defined 2a_0 periodicity along [1$\bar{1}$0]. The clean Si(5 5 7) surface also has wire structures with a 2a_0 periodicity at valley parts due to Si adatom rows [18]. However, their relative contrast in STM is significantly different from that observed on Ag/Si(5 5 7) (see the inset). This may indicate that the atomic structures of the ×2 atomic wires are different between the bare Si(5 5 7) and the Ag/Si(5 5 7) surfaces. The overall hill-and-valley morphology and the ×2 atomic wires observed here are fully consistent with the recent STM study [15]. The previous study further suggested that the ×2 atomic wires are metallic with a dispersing band crossing E_F based on the inverse photoemission data [15].

In addition to the hill-and-valley part, one can find two different minor domains (denoted as *A* and *B*) with less corrugations (Fig. 2a). Although these domains were not reported in the previous study [15], they always coexist with the major domain. Interestingly, the ×2 wire structures are also found in these domains.