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Tailoring of spin-split metallic surface-state bands on silicon

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ABSTRACT

To exploit Rashba effect in a two-dimensional electron gas on silicon surface for spin devices, it is necessary to have spin-split metallic surface-state bands. However, metals with strong spin-orbit coupling (e.g., Bi, Tl, Sb, Pt) induce reconstructions on silicon with almost exclusively spin-split insulating bands. We suggest to add a second adsorbate to these reconstructions in order to get spin-split metallic bands on silicon. The second adsorbate can affect the surface band structure in two ways. First, it can donate electrons to the available spin-split empty-state insulating or shallow metallic bands converting them to the well-defined metallic bands with enhanced electron filling. Corresponding example systems are Au/Si(1 1 1)$\sqrt{3}\times\sqrt{3}$ modified by In, Tl, Na or Cs and Tl/Si(1 1 1) modified by extra Tl adsorption. Second, by alloying a metal with a strong spin-orbit coupling with the other suitable metal one can obtain a dense two-dimensional alloy layer on silicon which electron band structure contains spin-split metallic bands. For example, this possibility was realized by alloying Bi/Si(1 1 1)$\sqrt{3}\times\sqrt{3}$ reconstruction with Na and Tl/Si(1 1 1)1×1 reconstruction with Pb. The suggested approach allows creation of the metallic surface-state bands with various spin textures on silicon and therefore enhances the possibility to integrate fascinating and promising capabilities of spintronics with current silicon-based technologies.

1. Introduction

The Rashba effect [1,2] which controls formation of a spin-polarized two-dimensional electron gas even in nonmagnetic materials is the key concept of many promising spintronics applications. For utilizing Rashba effect in semiconductor devices to be produced with the silicon-based technologies the requirements as follows have to be satisfied.

- The spin splitting should be large that would allow the device to operate at room temperature.
- The spin-split band should be metallic that would allow significant spin transport.
- The substrate should be a semiconductor that would allow the spin current to be detectable at the background of the non-polarized current through the substrate bulk. Silicon, the most widely used semiconductor material, seems to be the most suitable substrate.
- The layered nanostructure with desirable properties should be easily fabricated using the routine technique, e.g., molecular beam epitaxy.

Among the variety of the known systems with Rashba-type spin splitting of surface-state bands, the overwhelming majority fit only partially the above requirements. For example, the giant spin splitting was first detected on Bi-covered Ag(1 1 1) [3,4] but the substrate here is a metal. The spin-split metallic bands on a semiconductor were found first on Ge surface, namely on the Pb/Ge(1 1 1)$\sqrt{3}\times\sqrt{3}$ [5,6] and Au/Ge(1 1 1)$\sqrt{3}\times\sqrt{3}$ [7–9]. As for the Si substrate, a set of metal-induced reconstructions with Rashba splitting were found, including Bi/Si(1 1 1)$\sqrt{3}\times\sqrt{3}$ [10–12], Tl/Si(1 1 1)1×1 [13–15], Sb/Si(1 1 1)$\sqrt{3}\times\sqrt{3}$ [16] and Pt/Si(1 1 0)"6" $\times$ 5 [17] but in all the cases the spin-split surface-state bands were semiconducting. Thus, in order to create metallic spin-split bands on silicon one has to change somehow the band structure of the metal-induced Si reconstructions. Our suggestion is to employ a second metal adsorbate to reach this goal. As will be shown, a second adsorbate can affect the band structure in two ways. First, adsorbate-induced electron doping of the available insulating empty-state or shallow metallic bands can result in developing well-defined metallic bands with enhanced electron filling. Au/Si(1 1 1)$\sqrt{3}\times\sqrt{3}$ modified by Group-III or alkali metal

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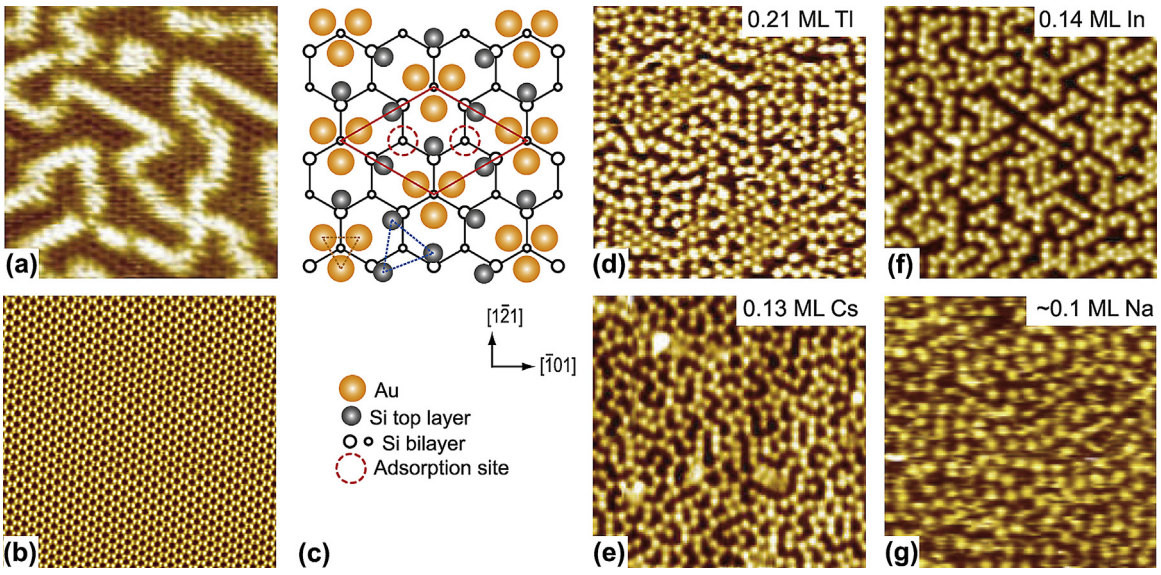

Fig. 1. Structural properties of adsorbate-modified Au/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ surface. Room-temperature STM images of the (a) pristine and (b) Tl-modified Au/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ surface. (c) CHCT model of the surfaces where Au atoms are shown by yellow circles, top Si atoms by gray circles, deeper Si atoms by white circles. Adsorption sites of the second adsorbate (In, Tl, Na or Cs) are outlined by dashed red circles. Low-temperature STM images of the Au/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ surface modified by adsorption of (d) Tl, (e) Cs, (f) In and (g) Na with indicated adsorbate coverage. Scale of all STM images is 170×170 Å^2. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

adsorbates and Tl/Si(1 1 1) modified by extra Tl adsorption set the examples. Second, interaction between two metal adsorbates might lead to the formation of a two-dimensional alloy with spin-split metallic bands. Several alloys demonstrating such properties (e.g., Bi–Na and Tl–Pb alloys on Si(1 1 1)) have already been found, the other are awaiting their discovery.

2. Experimental and calculation details

The STM and ARPES experiments were performed in an ultra-high-vacuum Omicron MULTIPROBE system with a base pressure better than $\sim 2.0 \times 10^{-10}$ Torr. Atomically-clean Si(1 1 1)7×7 surfaces were prepared in situ by flashing to 1280 °C after the samples were first outgassed at 600 °C for several hours. Pristine Au/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ surface was formed by Au deposition onto Si(1 1 1)7×7 surface held at ~600 °C. The adsorbate-modified Au/Si(1 1 1) surfaces were prepared by adsorbing 0.15 ± 0.05 ML (1.0 ML (monolayer) = 7.8×10^{14} cm^{-2}) of a given species, In, Na or Cs, onto the surface held at ~350 °C. Due to significant desorption, deposition of Tl was performed at room temperature (RT) followed by annealing at ~350 °C. Pristine Bi/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ and Tl/Si(1 1 1)1×1 reconstructions were formed by depositing 1.0 ML of the corresponding species onto Si(1 1 1)7×7 surface held at ~450 °C and ~300 °C, respectively.

STM images were acquired in a constant-current mode. Electrochemically-etched W tips and mechanically cut PtIr tips were used as STM probes after annealing in vacuum. ARPES measurements were conducted using VG Scienta R3000 electron analyzer and high-flux He discharge lamp ($h\nu = 21.2$ eV) with toroidal-grating monochromator as a light source.

Atomic structure of the alloyed (Bi, Na)/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ and (Tl, Pb)/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ reconstructions were elucidated using ab initio random structure search (AIRSS) technique [18] after it had been successfully tested for the known Bi/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ and Tl/Si(1 1 1)1×1 structures.

First-principles calculations were based on DFT as implemented in the Vienna ab initio simulation package VASP, [19,20] using a planewave basis and the projector-augmented wave approach [21] for describing the electron-ion interaction. The generalized gradient approximation (GGA) of Perdew, Burke, and Ernzerhof (PBE) [22] has been used for the exchange correlation potential. The Hamiltonian contains the scalar relativistic corrections, and the spin-orbit interaction was taken into account by the second variation method as has been implemented in VASP by Kresse and Lebacq [23]. To simulate the reconstructions we use a slab consisting of 12 bilayers. Hydrogen atoms were used to passivate the Si dangling bonds at the bottom of the slab. Both bulk Si lattice constant and the atomic positions within the three BLs of the slab were optimized including SOI self-consistently. The silicon atoms of deeper layers were kept fixed at the bulk crystalline positions.

3. Results and discussion

3.1. Adsorbate-induced modification of Au/Si(1 1 1) surface

Structural and electronic properties of the Au/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ surface have been the object of numerous studies. Its atomic arrangement is commonly accepted to be described by the conjugated honeycomb chained-trimer (CHCT) model [24,25]. In a larger scale, the main characteristic structural feature of the surface is a disordered meandering domain-wall network which separates the commensurate $\sqrt{3} \times \sqrt{3}$ domains [26] (Fig. 1a). Density of domain walls increases with Au coverage [26–28]. As for its electronic properties, the surface is known to be metallic [29], but its metallicity is not strongly expressed: the surface-state spectral features are smeared due to the domain walls and the metallic S_1 surface-state band is shallow, hence its electron filling is rather low, ~0.1 electrons per unit cell [30]. Therefore, though theoretical calculations [25,31] predict that the S_1 band is spin-split, this cannot be resolved in the experimental ARPES spectra from the pristine Au/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ surface [30].

However, poor structural and electronic properties of the Au/Si(1 1 1)$\sqrt{3} \times \sqrt{3}$ surface substantially improve after adsorbing small amounts of suitable species. This effect was found first for In adsorption [32] and then was spread to other adsorbates, namely Tl, Cs and Na [31,33]. The adsorbate-modified Au/Si(1 1 1) surfaces were prepared by adsorbing 0.15 ± 0.05 ML of a given species, In, Na or Cs, onto the surface held at ~350 °C. Due to significant

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