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Band structure of In chains on Si(335)–Au

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The crystallographic and electronic band structure of In induced reconstruction of Si(335)–Au surface have been studied with reflection high electron energy diffraction and angle resolved photoemission spectroscopy in ultrahigh vacuum conditions. The photoemission spectra recorded along chains show strongly dispersive band crossing the Fermi level while dispersionless spectra are found in the perpendicular direction. Diffraction experiments support one-dimensional character of the structures. A simple model of In reconstructed Si(335)–Au surface has been put forward.

Key words: one-dimensional structure; Si(335); In; ARPES; RHEED

1. Introduction

One-dimensional systems are very attractive objects for investigations because of their fundamental physical properties different from those of three- or two-dimensional systems, as well as for practical reasons consisting in rapid miniaturization of electronic components. Among many other metal–silicon systems, In–Si system has been studied for more than 40 years. Depending on In coverage and temperature, it reveals variety of reconstructions [1]. Among them there is 4×1 which shows a phase transition to 8×2 below 150 K, revealing one-dimensional character [2, 3]. Indium phases developed for submonolayer In coverages are found to be semiconducting, while those formed at around 1 monoatomic layer (ML), like 4×1 and $\sqrt{7}\times\sqrt{3}$ are metallic [1].

In the present paper, we report on investigation of In reconstructed Si(335)–Au vicinal surface. Electron diffraction and photoemission experiments show existence of one-dimensional metallic structures which are formed within submonolayer In coverages.

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2. Experimental

The experiments were performed under ultrahigh vacuum (UKV) with the base pressure of 7×10^{-11} mbar. The UHV system is equipped with a reflection high electron energy diffraction (RHEED) apparatus, an angle resolved photoemission spectroscopy (ARPES) setup, water cooled Au, In evaporators and quartz film thickness monitor. ARPES spectrometer consists of a helium lamp, an electron energy analyzer VGX900IC and a liquid nitrogen cooled manipulator which allows one to change both polar θ and azimuth φ angles.

In order to obtain Si(335) vicinal surface, p-type B-doped silicon was used. It was cut and oriented by means of X-ray diffraction technique with the accuracy of ±0.05°. Several flashes up to 1500 K in UHV were the final steps of substrate cleaning. In order to produce array of regularly distributed monoatomic steps 0.28 ML of Au was deposited on the surface kept at 900 K. 1 ML corresponds to 7.84×10^{14} atoms/cm^2 – the density of atoms in half of double layer of Si(111) plane. Subsequently, the substrate was annealed at 950 K for a few seconds and cooled to room temperature. Indium was deposited and annealed at 800 K for 60 s. During Au and In deposition, the pressure was in a high 10^{-11} mbar range. The whole sample cleaning and preparation procedures were controlled by RHEED.

In photoemission experiments, He I line (21.2 eV) with p-polarized radiation was used. Angular and energy resolution of the analyzer were fixed to 1.5° and 50 meV, respectively. Spectra were taken for two sample orientations, with step edges parallel and perpendicular to the plane of incident radiation. All measurements were performed at 120 K.

3. Results and discussion

Figure 1a shows a RHEED pattern of Si(335)–Au surface covered with 0.16 ML of In. The black spots denote high intensity diffracted beams associated with regularly

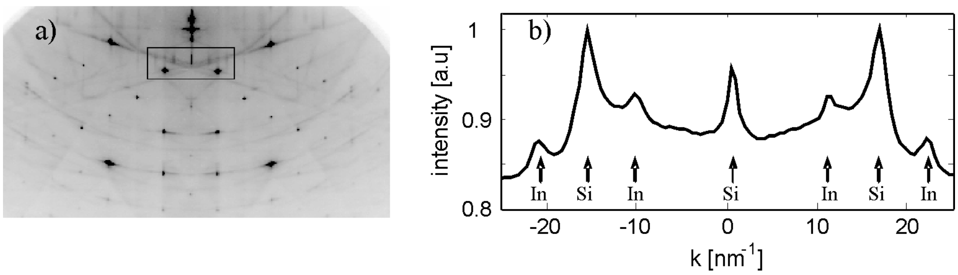

Fig. 1. RHEED pattern of Si(335)–Au surface covered with 0.16 ML of In and annealed at 800 K (a) and intensity profile taken from the marked region of a) (b); plane of incidence of the electron beam is perpendicular to the $[1\bar{1}0]$ direction

distributed monoatomic steps of Si(335)–Au substrate [4]. The presence of 0.16 ML of In deposited on that surface and annealed at 800 K is visible as additional, low intensity elongated streaks located between strong diffraction spots. They are much better visualized in the plot of intensity profile (Fig. 1 b), prepared from the marked region of the RHEED pattern. Indium induced peaks reach a broad maximum in the coverage range from 0.16 to 0.20 ML of In. The distance between neighbouring In and Si maxima Δk equals 5.43 nm^{-1} and corresponds to the period of $3a_{[1\bar{1}0]}$, where $a_{[1\bar{1}0]} = 0.384$ nm is the lattice constant along step edges.

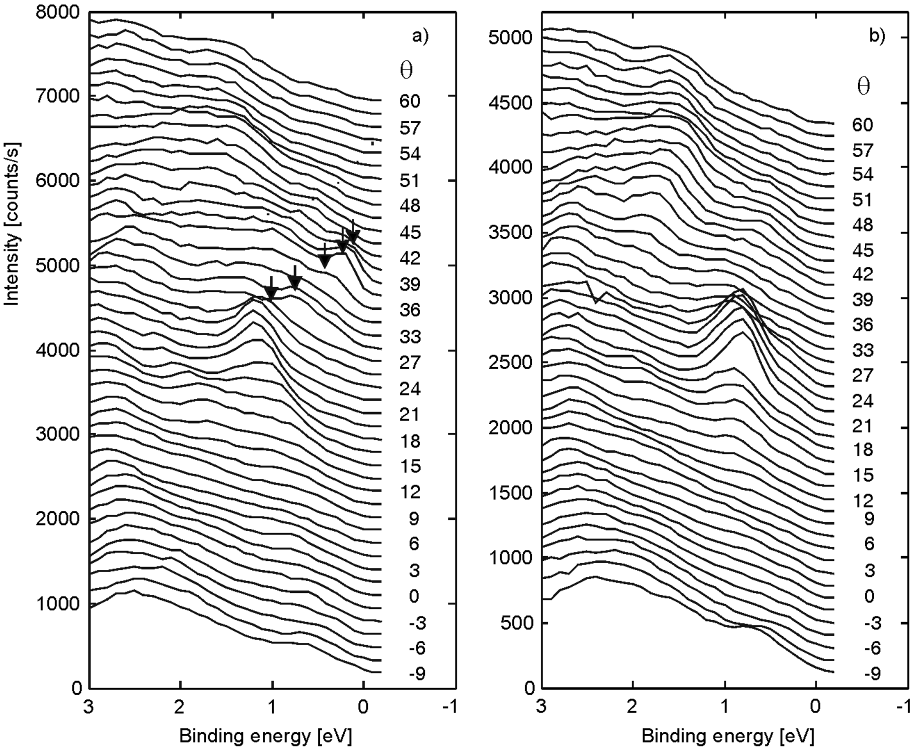

Fig. 2. ARPES spectra of: a) Si(335)–Au surface with 0.16 ML of In taken along step edges, b) bare Si(335)–Au. Spectra in Fig. 2a are shifted along intensity axis by a factor of 200 counts/s in order to prevent overlapping. Zero of binding energy denotes the Fermi energy. θ is an angle between surface normal and the entrance to electron energy analyzer. The arrows mark maxima which appeared after In deposition

Figure 2a shows ARPES spectra recorded for Si(335)–Au surface with 0.16 ML of In. The spectra were obtained for polar angle θ in the range from –9° to 60° every 1.5°, in the (110) plane parallel to the step edges of the substrate. The zero binding energy is at the Fermi energy, taken as the high kinetic energy threshold of the angle integrated spectrum. Figure 2b shows corresponding spectra recorded for Si(335)–Au substrate. Comparison of both sets of spectra shows that some of the features visible for the substrate are also present in the spectra of indium covered surface. This is the high intensity peak at about 1 eV and 24° which shifts toward higher binding energies by about 0.38 eV after covering the surface with In. Other bands associated with bulk silicon are also visible at higher binding energies. A peak located at about 0.9 eV and 27° which moves toward the Fermi energy with increasing θ and approaches E_F at about 39° is a new feature found in the spectra of In covered surface.

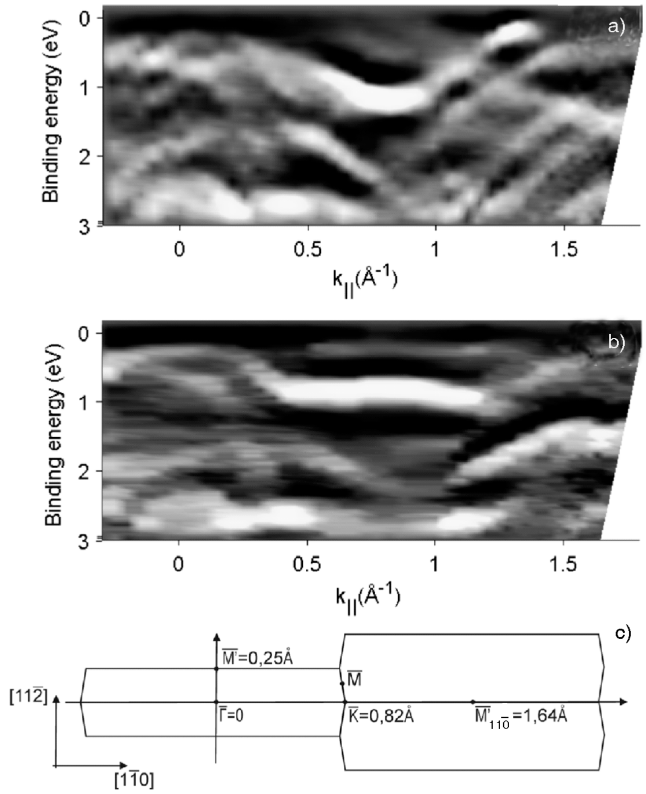

Fig. 3. Map of the second derivative of fotoemission intensity for In covered (a) and bare Si(335)–Au (b) surfaces; c) the surface Brillouin zone of Si(335) surface. The momentum component $k_{||}$ is parallel to the $[1\bar{1}0]$ direction

A very convenient way for presentation of ARPES spectra is displaying them as a map of the second derivative of photoemission intensity versus binding energy and wave vector component $k_{||}$. This procedure enhances weak features of acquired spectra. The result is shown in Fig. 3 for In covered (a) and bare (b) Si(335)–Au surfaces. The momentum component $k_{||}$, parallel to the $[1\bar{1}0]$ direction, spans over two Brillouin zones of the Si(335) surface (Fig. 3c). A minimum of highly dispersive band is located at $\bar{K}$ point and the band crosses the Fermi level at about 1.37 Å^{-1}, indicating a metallic character of the investigated system.

Photoemission spectra recorded across the step edges show no dispersive bands close to the Fermi level revealing one-dimensional character of the system. This is shown in Fig. 4 where two exemplary spectra, along (upper) and across (lower) the step edges, recorded at the same θ of 42°, are plotted.

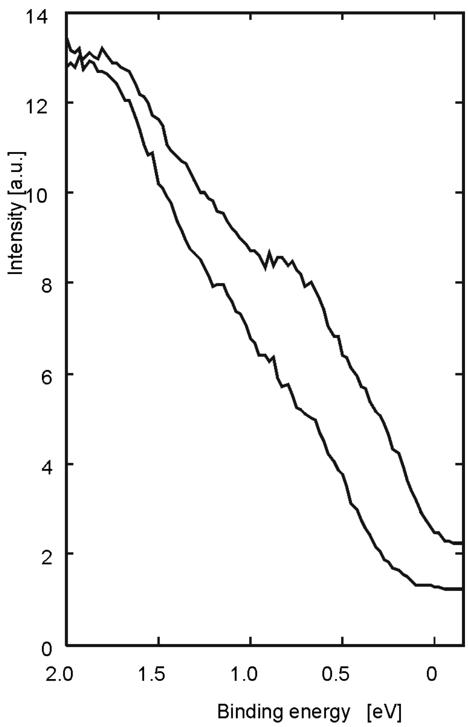

Fig. 4. ARPES spectra for $\theta = 42°$ along (upper curve) and across (lower curve) In chains

The unit cell of Si(335)–Au surface has a size of $\mathbf{1}a_{[1\bar{1}0]}\times 3(2/3)a_{[11\bar{2}]}$. Filling each unit cell with a single In atom requires coverage of 0.27 ML. The $3\times a_{[1\bar{1}0]}$ periodicity for coverages of 0.16 to 0.20 ML observed in RHEED experiment suggests an average occupancy of 2 In atoms per 3 unit substrate cells. This gives (2/3)×0.27 ML = 0.18 ML as an ideal coverage. Since unreconstructed Si(335) surface is composed of (111) terraces, some suggestions might be found in experiments on a flat Si(111) surface. For example the (4×1)-In reconstruction shows one-dimensional and simultaneously metallic character, but that reconstruction occurs at coverage of about 1 ML and temperatures below 450 °C [1, 5]. Within the temperature and coverage ranges studied in the experiments reported in this paper, the only possible reconstruction that can exist on a flat Si(111) surface, is the $(\sqrt{3}\times\sqrt{3})$ In [5] with the saturation coverage of 1/3 ML, which gives one In atom per $(\sqrt{3}\times\sqrt{3})$ unit cell [5].

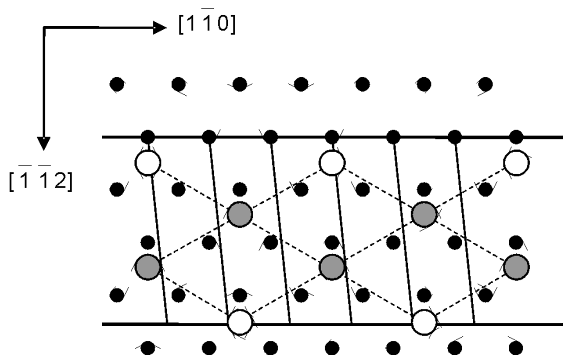

Fig. 5. Top view of unreconstructed Si(111) surface with marked $\sqrt{3}\times\sqrt{3}$ unit cells (dashed lines) and In adatoms (large circles). The horizontal lines define the width of (111) terrace of (335) surface. Several unit cells of (335) surface are also marked

Figure 5 shows a top view of (111) surface with marked several ($\sqrt{3}\times\sqrt{3}$) unit cells (dashed lines). Large circles indicate In atoms located at the T_4 sites [6]. Two horizontal lines indicate the $[1\bar{1}0]$ direction and might be thought as a position of step edges defining a (111) terrace of the (335) surface. Several unit cells of the (335) surface are also marked. There are three rows of In atoms which fit to the width of (111) terrace and one row at its edge. The coverage of 0.18 ML denotes the number of In atoms which are in two rows. There are many possibilities of arranging In atoms in a way to get $3a_{[1\bar{1}0]}$ periodicity. One of the possibilities is to remove two chains and leave the other two as they exist in the ($\sqrt{3}\times\sqrt{3}$) superstructure (e.g., shaded circles).

The arrangement of In atoms into zig-zag chain structure supports one-dimensional character of the grown structures shown by ARPES experiments. The smallest distance between indium atoms in a row, equal to $\sqrt{3}a_{[1\bar{1}0]}$, seems to be too large to be responsible for the observed in ARPES experiment metallic behaviour. The observed metallicity should be rather explained as a charge transfer to the substrate, possibly to Au monoatomic chain, and creation of an “effective” metallic chain as in the case of Pb on Si(335)–Au [7]. Trivalent In atoms act as donors what also explains the observed decrease of work function by about 0.15 eV and shift of bands to a higher binding energy.

4. Summary

Crystallographic and electronic structures of In reconstructed Si(335)–Au surface have been investigated. We found that 0.16 ML of In annealed at 800 K on the Si(335)–Au surface creates one-dimensional and metallic chains. A simple model explaining observed features has been proposed which assumes a new surface unit cell of $3a_{[1\bar{1}0]} \times 3(2/3)a_{[11\bar{2}]}$ consisting of 2 In and 3 Au atoms inside. Such a simple model does not define exact position of In atoms on (111) terraces and certainly more studies, especially STM, are needed.

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