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Tb silicide nanowire growth on planar and vicinal Si(001) surfaces

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ABSTRACT

Scanning tunneling microscopy and low energy electron diffraction were used to investigate the growth of Tb silicide nanowires on Si(001) and its dependence on Tb coverage, annealing temperature, and the vicinality of the substrate. The nanowires are observed both isolated and in bundles, and while being narrower than 4 nm, they reach lengths exceeding 500 nm. Their appearance fits a hexagonal $TbSi_2$ structure model with Si dimer rows on top of the nanowires. The growth of exclusive parallel nanowires was achieved on vicinal surfaces. On planar samples, the nanowire growth is accompanied by the formation of a 2×7 reconstruction that shows a wetting layer like behavior. In contrast, mainly building blocks of this 2×7 reconstruction are observed on vicinal samples.

1. Introduction

In 1998, the first observation of rare earth (RE) silicide nanowires was reported by Preinesberger et al., who studied Dy induced surface structures on Si(001) by scanning tunneling microscopy (STM) [1]. Two years later, Chen et al. explained the growth of Er silicide nanowires with the assumption that they consist of hexagonal $ErSi_2$ [2]. This silicide fits structurally well on the unreconstructed Si(001) surface with a nearly perfect lattice match along its *a*-axis, but a high lattice mismatch along its *c*-axis. Thus, the growth of highly elongated islands is promoted, so that nanowires form. Based on this structural model, Chen et al. proposed the formation of nanowires for various other trivalent RE metals that form hexagonal $RESi_2$ [3]. Indeed, nanowire formation was observed for all but two of these trivalent RE metals [3–6]. Firstly, Sm does not induce nanowires on Si(001) due to a rather high mismatch even along the silicide *a*-axis [4]. Secondly, the existence of Tb silicide nanowires was never investigated up to now, to the best of our knowledge.

Despite the chemical similarities of the various trivalent RE metals, the properties of RE silicide nanowires vary. Some differences can be traced back to differences of the bulk RE disilicides, e.g. slightly different lattice parameters result in a variation of the observed average nanowire widths [3]. Other differences are not understood up to now: While all nanowires studied by scanning tunneling spectroscopy or by angle resolved photoelectron spectroscopy are metallic at room temperature, an electronlike band crossing the Fermi Energy was observed around the $\bar{\Gamma}$ point for $ErSi_2$ and $DySi_2$ nanowires but not for $GdSi_2$ nanowires [5,7–11]. Moreover, a 2×7 reconstructed superstructure, which may cover the surface between the nanowires forming a wetting layer, was found for most RE metals inducing nanowire formation, but not for Er [6,7,9,12–14].

This 2×7 reconstruction was found to be insulating, so that the growth of electrically well isolated nanowires required for applications is possible when this reconstruction forms [11]. Possible applications of the nanowires include the use as nanoscale interconnects due to their metallicity, eventually enabling a further miniaturization in electronics. They are especially interesting in this respect since they grow on the Si(001) surface being the main substrate used for semiconductor electronics. Also other applications in discussion for one-dimensional metals, e.g. as plasmonic waveguides, might be feasible [15].

Furthermore, the $RESi_2$ nanowires are not only interesting for applications, but also promising candidates for investigating unique phenomena of one-dimensional metals, e.g. the Tomolga Luttinger liquid behavior or Peierls transitions [16–19]. Indeed, indications for a Peierls transition were found at low temperatures for YSi_2 nanowires [5]. Interestingly, $GdSi_2$ nanowires showed no Peierls transition down to even lower temperatures [9]. Thus, also the observation of one-dimensional phenomena seems to be strongly dependent on the investigated RE silicide.

Here, we report on the formation of Tb induced structures on Si(001) surfaces, closing the knowledge gap regarding the existence of $TbSi_2$ nanowires and focusing on a detailed growth analysis. We largely varied the Tb coverage and the post deposition annealing temperature in order to obtain an overview on the forming structures. The samples were investigated *in-situ* by STM and low energy electron diffraction (LEED). Thereby, we found not only nanowires and bundles of nanowires, but also a 2×7 reconstruction and large, well defined islands. The nanowires and the 2×7 reconstruction were further analyzed in detail and their interplay during the nanowire formation was studied in

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depth. Moreover the growth of exclusively parallel nanowires was demonstrated on vicinal Si(001) surfaces.

2. Experimental details

Planar and vicinal Si(001) samples were cut from *n*-type and *p*-type Si wafers. The samples were resistively heated, and their temperature was controlled using an infrared pyrometer (accuracy ±20 °C). They were outgassed in ultra-high vacuum at 800 °C for several hours and subsequently flash heated repeatedly to 1150 °C to desorb the Si oxide layer and other contaminants. To achieve well ordered surfaces, the samples were then slowly cooled down from around 850 °C to room temperature. The success of this initial cleaning was controlled by STM for every sample.

Tb was evaporated from a homebuilt electron-beam evaporator. The Tb flux was controlled prior to the Tb deposition by a quartz-crystal microbalance (accuracy ±20%) situated at the sample position. The Tb coverage, given in monolayers (ML), was determined by the deposition time and ranged from 0.25 ML to 2.20 ML. 1 ML corresponds to one deposited Tb atom per Si surface atom, i.e. 6.8×10^{14} atoms/cm^2. After the Tb deposition at room temperature, the samples were annealed at temperatures between 400 °C and 700 °C for 2 min to enable the silicide formation. The pressure in the preparation chamber, which also contains the LEED system, did not exceed 3×10^{-9} mbar during the entire preparation process, while the base pressure was below 5×10^{-10} mbar. LEED images were obtained by taking pictures of the LEED screen using a CCD camera. They are shown with inverted contrast and rotated to fit the orientation of the STM data when necessary.

The used room temperature STM is homebuilt and situated in an additional chamber with a pressure below 1.5×10^{-10} mbar. The STM images were taken in constant current mode with sample voltages (V_T) between −2.5 V and +2.5 V and typical tunneling currents of 100 pA to 1 nA. The STM tips consist of chemically etched W wires, which were *in-situ* cleaned by heating with electron bombardment. All STM images were analyzed and processed using the wsxm software [20]. In some cases the real image was superposed with its derivative to highlight height variations within shallow structures.

3. Results and discussion

There are four different wire-like structures that may be induced by Tb on Si(001) surfaces: single nanowires, nanowire bundles, the 2×7 reconstruction, and dark wires. In Fig. 1(a) single nanowires and nanowires bundles are the most prominent features, but, additionally, there are faint rows due to 2×7 reconstructed patches. Such a 2×7 reconstruction is shown in detail in Fig. 1(b) together with the fourth wire-like structure, the dark wires.

These dark wires are considered an intermediate state between the 2×7 reconstruction and the nanowires and may be observed in particular for low annealing temperatures [21]. They are wider and appear less structured and higher than the 2×7 reconstruction, but have an apparent height lower than a monoatomic substrate step, in contrast to the nanowires [see Fig. 1(b)].

In this work, we will focus on single nanowires, nanowire bundles, and the 2×7 reconstruction. These structures are analyzed in depth and their growth behavior and interaction will be discussed in detail during the course of this report. Beforehand, we want to find out, on which parameter range we have to focus to observe these structures dominantly.

3.1. Influence of the growth parameters

Figs. 2(a, b) show an STM image and a LEED pattern of a clean, planar Si(001) surface. This surface is characterized by Si dimers and monoatomic steps. The Si dimers form a 2×1 reconstruction at room temperature as can be verified by the LEED image where ×2 spots are seen. These spots show up in [110] and [$\bar{1}$10] direction since the 2×1 reconstruction rotates by 90° on neighboring terraces resulting in two different domains. This rotation can be nicely seen in STM images, where the 2×1 reconstruction appears in form of Si dimer rows [see Fig. 2(a)], and also leads to a rotation of the Tb induced structures on neighboring terraces as can be observed in Fig. 1. Furthermore, there are two different types of step edges. If the Si dimer rows on the upper terrace are parallel (perpendicular) to the step edge, straight (rough) step edges form [22].

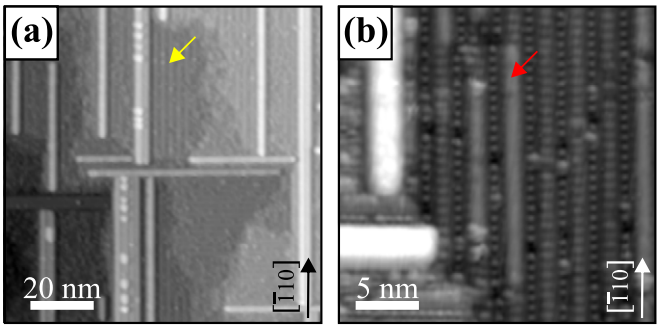

Fig. 1. (a) Filled states STM image of the nanowire growth on a planar Si(001) surface (0.50 ML Tb annealed at 600 °C, $V_T = -1.5$ V). The yellow arrow indicates a 2×7 reconstructed patch. (b) Filled states STM image of a surface area covered with the 2×7 reconstruction, two nanowires, and dark wires, one of the latter is marked by the red arrow (0.70 ML Tb annealed at 500 °C, $V_T = -1.5$ V).

Depositing 0.40 ML Tb on a clean Si(001) surface without annealing leads to the surface morphology as seen in Fig. 2(c). Straight and rough step edges are still found, but no features directly related to Si dimer rows can be observed any more. Small, cluster-like accumulations are randomly distributed across the surface. They do not show any

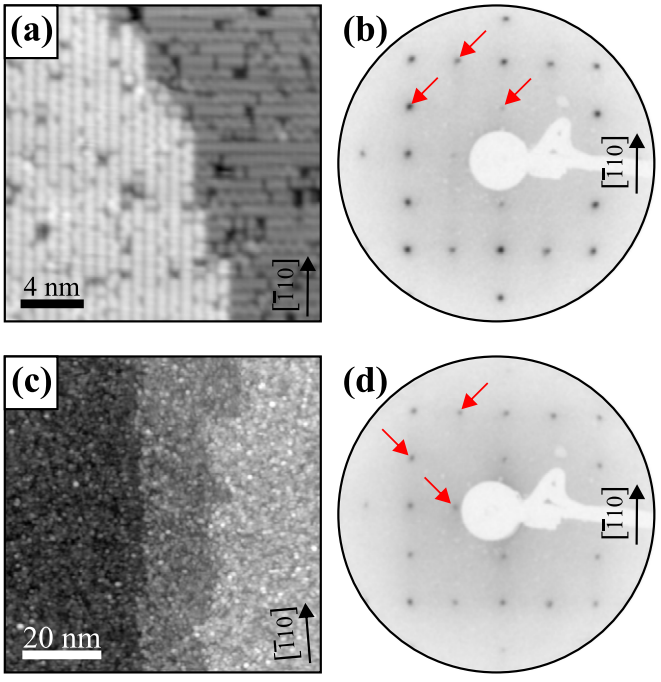

Fig. 2. (a) STM image ($V_T = -1.5$ V) and (b) LEED image ($E_{kin} = 50$ eV) of a clean Si(001) surface. Some ×2 spots characteristic for a two domain 2×1 reconstruction are marked by red arrows. (c) STM image of a Si(001) surface with 0.40 ML Tb without post deposition annealing ($V_T = -1.5$ V). (d) LEED image of a Si(001) surface covered with 0.75 ML Tb without post deposition annealing ($E_{kin} = 50$ eV).