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Atomically precise self-assembly of one-dimensional structures on silicon

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Abstract

This work has three main themes: (1) fabricate atomically precise nanostructures at surfaces, particularly nanowires consisting of atom chains; (2) explore the behavior of one-dimensional electrons in atomic chains; (3) find the fundamental limits of data storage using an atomic scale memory. Semiconductor surfaces lend themselves towards self-assembly, because the broken covalent bonds create elaborate reconstruction patterns to minimize the surface energy. An example is the large 7×7 unit cell on Si(1 1 1), which can be used as building block. On semiconductors, the surface electrons completely de-couple from the substrate, as long as their energy lies in the band gap. Angle-resolved photoemission reveals surprising features, such as a fractional band filling and a spin-splitting at a non-magnetic surface. An interesting by-product is a memory structure with self-assembled tracks that are five atom rows wide and store a bit by the presence or absence of a single silicon atom. This toy memory is used to test the fundamental limits of data storage and to see how storage on silicon compares to storage in DNA.

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1. Introduction

Nanostructures can be produced by two generic methods, lithography and self-assembly. Lithography becomes more difficult for smaller structures, while self-assembly becomes easier. Below a certain size, it is possible to produce atomically precise structures. This regime will be explored in the following. A particularly interesting aspect is the assembly of atomic chains at surfaces [1]. These come close to the ideal nanowire, an infinite chain of atoms freely suspended in space. Such a wire is nearly impossible to produce experimentally. Free-standing chains of metal atoms can be sustained up to about four atoms in length [2–4], but they are rather unstable. As we will show in the following, it is possible to form rigid atom chains at vicinal Si(1 1 1) surfaces, which combine the best of two worlds: the atoms are firmly locked to the surface (usually in substitutional silicon atom sites). The metallic electrons, on the other hand, are de-coupled from the silicon substrate. There are no bulk states in the band gap that could hybridize with the surface states. A large variety of such atomic chain structures has been discovered in recent years, which provide a new playground for exploring the physics of electrons as they approach the one-dimensional limit.

One-dimensional physics is particularly simple and elegant. Many problems can be solved analytically. Some problems involving highly correlated electrons can only be solved at all in one dimension. Whole books have been written about this topic [5,6]. One of the peculiar features of electrons in one dimension is the breakdown of the single-electron picture. Theory predicts that the single-electron picture breaks down in a one-dimensional solid. This statement can be rationalized rather simply: electrons cannot avoid each other when moving along the same one-dimensional line. A single excited electron creates a domino effect by colliding with a nearby electron, which collides with the next electron, and so on. This strong interaction has startling consequences on the physics of one-dimensional systems leading to a variety of unusual phases at low temperatures. The most striking prediction is the breakup

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of electrons into separate spin and charge excitations, the spinons and holons [5]. A variety of other interesting phases exist for one-dimensional systems, such as Peierls-insulators, charge density waves, spin density waves, singlet and triplet superconductivity, and so on [6].

2. Self-assembly of one-dimensional structures

The ever-increasing sophistication in the preparation of single crystal surfaces has made it feasible to tailor surfaces in many ways. The arrival of scanning tunneling microscopy has provided a much more critical look at the perfection of surfaces than diffraction methods, which emphasize the ordered part of the surface. That has helped controlling surfaces more precisely and producing large areas of defect-free surfaces. One-dimensional structures can be prepared by using stepped surfaces as templates. Particularly well suited are surfaces with large unit cells, such as Si(1 1 1)7 × 7 and Au(1 1 1). The steps become very straight in this case, because the formation of a kink requires adding many extra atom rows, for example 2 × 7 = 14 rows for Si(1 1 1)7 × 7. As a result, atomically straight step edges with a length of 20,000 edge atoms have been achieved on Si(1 1 1)7 × 7 by a simple sequence of anneals [7,8]. This requires of course an accurate azimuthal cut of the Si wafer. The length of kink-free terraces can be extended by heating the wafer with DC current parallel to the steps and keeping it strain-free during heating. A current parallel to the steps causes bunching of the kinks into large facets due to electromigration [9,10].

The step spacing can be controlled by taking advantage of the step–step interaction via their strain field [11]. A repulsive step–step interaction favors equi-spaced steps. The steps need to spaced together closely to provide an interaction large enough for an atomically perfect step spacing. This happens for vicinal Si(1 1 1) at a step spacing of about 6 nm, as shown in Fig. 1 (from [12]). This Si(5 5 7)3 × 1 surface structure consists of a triple step and a terrace containing a single 7 × 7 unit cell. The period of this atomic scale grating is known very accurately since the lattice constant of Si is a secondary length standard (compare the number of significant digits given in Fig. 1). Such structures are being studied as possible length standards in the nanoscale regime, which are important for getting an accurate overlay in lithography of microelectronic devices. While lithography becomes more difficult when pushing towards smaller dimensions, self-assembly becomes easier. Bridging the gap between self-assembly and lithography and combining the best of both methods has become an important goal for nanotechnology. Here we are concerned with pushing atomically precise self-assembly to larger dimensions. The 6 nm period in Fig. 1 is typical of the largest structures that can be obtained at surfaces with atomic perfection of wide areas. The building blocks for such structures are typically 50 atoms in size, for example the 7 × 7 unit cell, the C_{60} fullerene, and the ''magic'' Au_{55} cluster. It will be interesting to see whether the size of perfectly self-assembled structures can be increased. Another alternative would be a directed assembly process, where a coarse grid is defined by lithography (either conventional optical lithography or EUV interference lithography [13]) and then filled in by self-assembly.

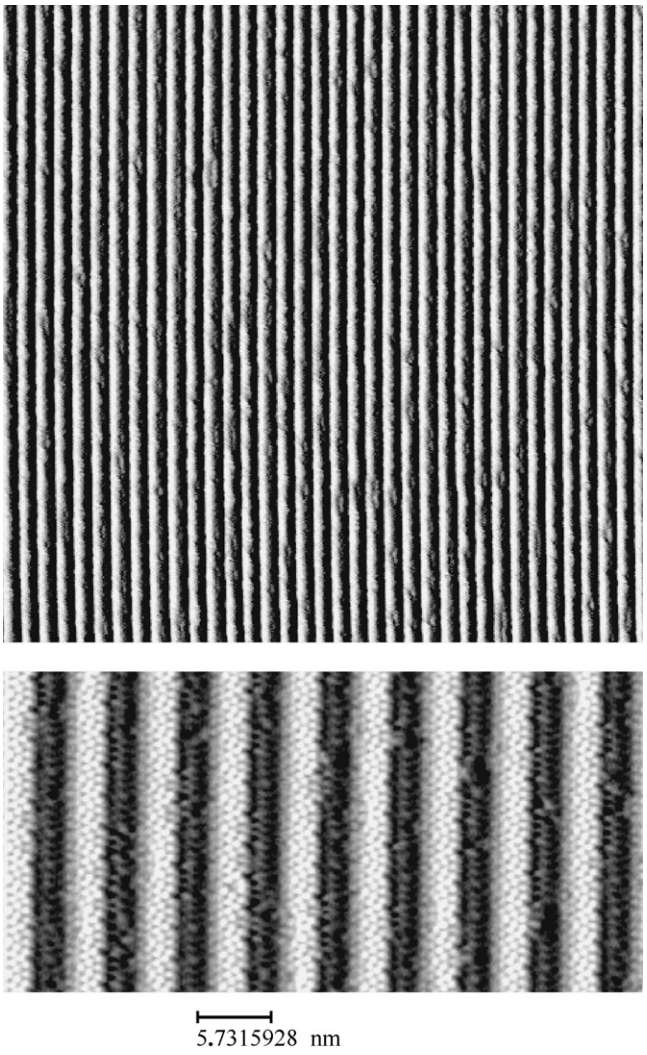

Fig. 1. Step structure created on Si(5 5 7), a vicinal Si(1 1 1) surface. Atomic perfection is achieved by using the large Si(1 1 1)7 × 7 unit cell as building block (bright stripes) and having the steps close enough to strongly interact with each other. This, and all following STM images show the derivative of the topography in the *x*-direction, which gives the impression of illumination from the left. From [12].

Stepped surfaces can be converted into atomic chain structures by depositing a sub-monolayer of metal atoms, most notably gold [1]. Typical growth parameters are a substrate temperature of 600–700 °C during Au deposition and a subsequent post-anneal to 800–900 °C for a few seconds with slow cool-down over several minutes. An example is given in Fig. 2a, where the Si(5 5 7) surface from Fig. 1 is converted to a chain structure by 0.2 of a monolayer of Au. This method works for a large group of metal atoms (alkalis, alkaline earths, In, Ag, Au, Pt, and rare earths). These comprise valence states from 1 to 3, s-, p-, d-, and f-electrons, and magnetic atoms. Even the flat Si(1 1 1) surface forms one-dimensional chain structures with three domains. A single domain can be selected by choosing a small miscut of about 1–2°. Apart from the Si(1 1 1) surface, which has the advantage of a large unit cell, there are several