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### Authors

Ragan, Regina

Chen, Yong

Ohlberg, Douglas AA

et al.

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# Ordered arrays of rare-earth silicide nanowires on Si(0 0 1)

Regina Ragan<sup>a,\*</sup>, Yong Chen<sup>a</sup>, Douglas A.A. Ohlberg<sup>a</sup>,  
Gilberto Medeiros-Ribeiro<sup>b</sup>, R. Stanley Williams<sup>a</sup>

<sup>a</sup>Quantum Science Research, Hewlett-Packard Laboratories, 1501 Page Mill Road, MS 1123, Palo Alto, CA 94304, USA

<sup>b</sup>LNLS—Laboratorio Nacional de Luz Sincrotron, R. Giuseppe Maximo Scolfaro 10000, 13083-360 Campinas, SP, Brazil

## Abstract

Ordered arrays of self-assembled  $\text{ErSi}_{2-x}$ ,  $\text{SmSi}_{2-x}$ , and  $\text{DySi}_{2-x}$  nanowires aligned along Si [1 1 0] have been grown at 600°C on Si(00 1) vicinal substrates. The nanowires grow perpendicular to the Si dimer rows and are 1.5–5 nm wide, approximately 2 monolayers high and up to 1 μm long. These nanowires were characterized in situ with scanning tunneling microscopy.

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## 1. Introduction

Many rare-earth silicides ( $\text{RSi}_{2-x}$ , with  $x \sim 0.30$ ) [1] with the  $\text{AlB}_2$  (hexagonal) crystal structure have been demonstrated to self-assemble into one-dimensional nanostructures during epitaxial growth on Si(1 1 1) and Si(0 0 1) [2–5]. On Si(1 1 1) substrates,  $\text{RSi}_{2-x}$  nanowires grow along the [1 1 0] step edges [6]. Alternatively, the evolution of the one-dimensional structure during epitaxial growth on Si(0 0 1) has been attributed to an anisotropic lattice mismatch between the [1 1  $\bar{2}$  0] and [0 0 0 1] lattice constants of the  $\text{RSi}_{2-x}$  and the Si [1 1 0] lattice constant,  $a_{\text{Si}[1 1 0]}$  [2]. The  $\text{RSi}_{2-x}$  grows preferentially in the direction that

has the lowest lattice mismatch with  $a_{\text{Si}[1 1 0]}$ , thus, forming nanowires. Two orientations of nanowires grow on ‘flat’ Si(0 0 1) substrates with the long axes of the nanowires orthogonal to one another and perpendicular to the Si dimer rows. In this paper, we demonstrate the alignment of  $\text{RSi}_{2-x}$  nanowires along a single direction. Self-assembled  $\text{ErSi}_{2-x}$ ,  $\text{SmSi}_{2-x}$  and  $\text{DySi}_{2-x}$  nanowires aligned along Si[1 1 0] were grown on vicinal Si(0 0 1) substrates with aspect ratios exceeding 100 and feature heights on the order of a few monolayers (ML). The microstructure was characterized in situ with scanning tunneling microscopy (STM). The low coverage regime was studied to gain insight into the mechanism behind nanowire nucleation and alignment.  $\text{RSi}_{2-x}$  nanowires may have applications as non-lithographically fabricated small-scale interconnects. In addition, one-dimensional structures may exhibit interesting

\*Corresponding author. Tel.: +1-650-236-4515; fax: +1-650-813-3312.

E-mail address: [regina.ragan@hp.com](mailto:regina.ragan@hp.com) (R. Ragan).

phenomenon such as a Peierls transition [7] and Luttinger liquid behavior [8]; hence, characterization of  $\text{RSi}_{2-x}$  nanowires may lead to a deeper fundamental understanding of the physical properties of one-dimensional structures.

## 2. Experiment

$\text{Si}(001)$  vicinal substrates with a miscut of  $2.5^\circ$  toward  $[110]$  were prepared by heating the substrate to a temperature of  $1150^\circ\text{C}$  for 15 s in ultrahigh vacuum with a chamber pressure  $< 1 \times 10^{-9}$  Torr. The  $\text{Si}(001)$  surface was analyzed in situ with a STM to ensure a clean surface prior to deposition. Physical vapor deposition of elemental rare-earth materials was performed via an electron beam evaporator. The growth rate of the rare-earth material was  $\sim 0.1$  ML/min and the substrate temperature during deposition was  $600^\circ\text{C}$ . The sample was annealed post-growth at  $600^\circ\text{C}$  to drive the reaction between the rare-earth element and Si to completion. The nanowires were characterized in situ with an Omicron STM with a chamber pressure  $< 2 \times 10^{-10}$  Torr.

## 3. Results and discussion

STM images of  $\text{ErSi}_{2-x}$  and  $\text{SmSi}_{2-x}$  nanowire arrays oriented along  $\text{Si}[110]$  are seen in Figs. 1(a) and (b), respectively. The imaged region,  $1 \times 1 \mu\text{m}^2$ , illustrates the high aspect ratio of these

nanowires. The  $\text{ErSi}_{2-x}$  nanowire marked with an arrow in Fig. 1(a) has a length exceeding  $1 \mu\text{m}$  and the  $\text{SmSi}_{2-x}$  nanowire similarly marked in Fig. 1(b) has a measured length of 750 nm. The width of the  $\text{ErSi}_{2-x}$  nanowire, seen in Fig. 2(a), has a measured value of 4.7 nm and the height was measured as 0.7 nm. Shown in Fig. 2(b), the  $\text{DySi}_{2-x}$  nanowires have a measured average width of 2 nm, a measured height of 1 nm, and the average distance between the nanowires is 9 nm. In comparison, the  $\text{SmSi}_{2-x}$  nanowires, shown in Fig. 2(c), have an average measured width of 1.5 nm and a height of approximately 0.6 nm. The lattice mismatch between  $\text{Si}[\bar{1}10]$   $\{\text{Si}[110]\}$  and  $\text{ErSi}_{2-x}$ ,  $\text{DySi}_{2-x}$ , and  $\text{SmSi}_{2-x}$   $[0001]$   $\{[11\bar{2}0]\}$  is 6.3%  $\{-1.6\%$ , and 7.6%  $\{-0.1\%$ , and 9.8% and  $\{1.6\%$ , respectively. In agreement with previous work [3], the nanowire width decreases with increasing lattice mismatch between the  $\text{Si}[\bar{1}10]$  and  $\text{RSi}_{2-x}$   $[0001]$  lattice constants.

$\text{Si}(001)$  substrates with a miscut  $< 2^\circ$  have single atomic steps and the terraces alternate between dimer rows running parallel (type A) and perpendicular (type B) to the step edge. Since the nanowires grow perpendicular to the Si dimer rows, growth on flat  $\text{Si}(001)$  substrates produces  $\text{RSi}_{2-x}$  nanowires oriented in two orthogonal directions [3]. The Si terraces retreat from an advancing nanowire and form step bunches [2]. Nanowire growth is terminated after intersection with another nanowire or after the nanowire has burrowed into a limited number of terraces [2]. Thus, a  $\text{Si}(001)$  template having double atomic

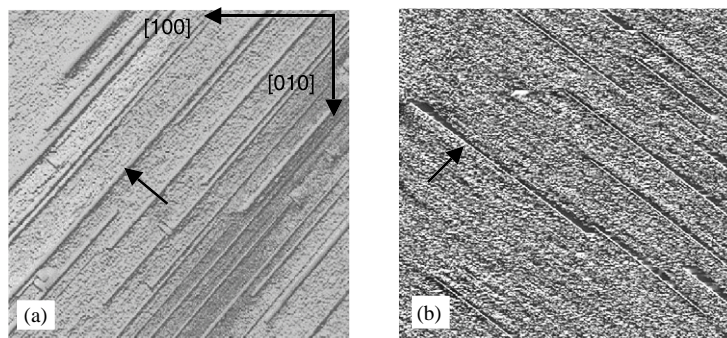


Fig. 1. STM images having a  $1 \times 1 \mu\text{m}^2$  scan region of (a)  $\text{ErSi}_{2-x}$  and (b)  $\text{SmSi}_{2-x}$  nanowire arrays on vicinal  $\text{Si}(001)$  substrates with a miscut of  $2.5^\circ$  toward  $[110]$ . The  $\text{RSi}_{2-x}$  nanowire arrays are oriented along the  $\text{Si}[110]$  direction. The  $\text{ErSi}_{2-x}$  ( $\text{SmSi}_{2-x}$ ) nanowire indicated by the arrow has a measured length exceeding  $1 \mu\text{m}$  (750 nm).

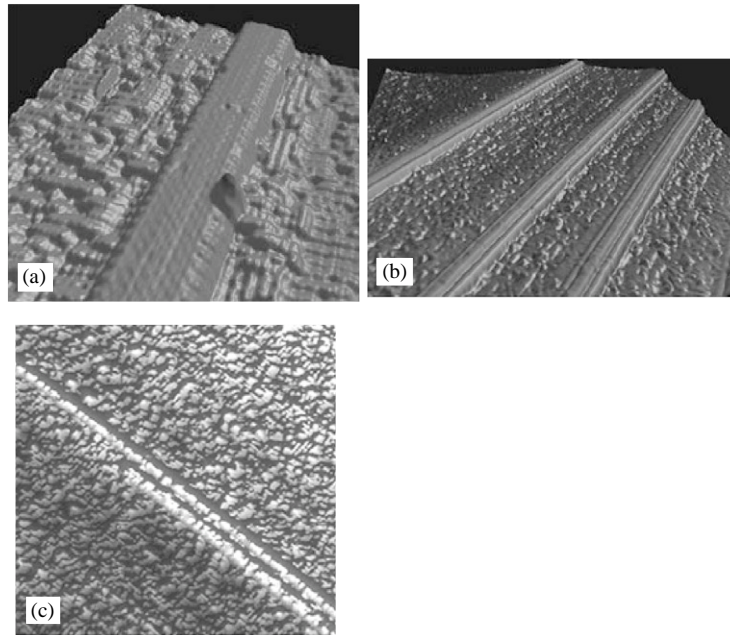


Fig. 2. High-resolution STM images of (a)  $\text{ErSi}_{2-x}$  nanowires with wire width of 4.7 nm and height of 0.7 nm, (b)  $\text{DySi}_{2-x}$  nanowires where the width is 2 nm, the height is 1 nm and the average distance between the nanowires is 9 nm, and (c)  $\text{SmSi}_{2-x}$  nanowires with wire width of 1.5 nm and height of 0.7 nm.

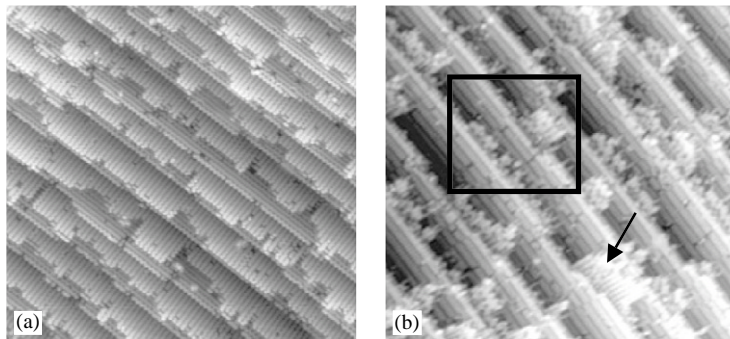


Fig. 3. STM images having a  $50 \times 50 \text{ nm}^2$  scan region of (a) a  $\text{Si}(001)$  vicinal substrate with  $2 \times 1$  surface reconstruction and double atomic steps of type B and (b) the Si surface with low Sm coverage. The arrow points to a region where Si dimer rows are still visible on the surface.

steps of type B is necessary for epitaxial growth of nanowire arrays oriented parallel to the step edge, thereby, having a high length-to-width aspect ratio. In Fig. 3(a), an STM image of the  $\text{Si}(001)$  vicinal surface with a miscut of  $2.5^\circ$  toward  $[110]$  portrays a  $2 \times 1$  reconstructed surface consisting of double atomic steps of type B. The low coverage regime,  $<0.15 \text{ ML}$ , was investigated to probe

nanowire nucleation. Atomic strings have been observed in STM images of Er [9], Dy [10], and Sm and may serve as nuclei for nanowire growth. In Fig. 3(b), a  $50 \times 50 \mu\text{m}^2$  STM image of the Si surface with low Sm coverage is shown. New features, oriented perpendicular to the Si dimer rows, appear. The  $20 \times 20 \text{ nm}^2$  region in the square of Fig. 3(b) is shown in Fig. 4(a). A line profile

taken across the line in the upper left corner of this STM image, shown in Fig. 4(b), resolves two peaks in each row indicating these new features are dimers on the surface. The periodicity of these dimer rows was measured as 1.2 nm. This periodicity is 1.5 times the observed periodicity, 0.8 nm, of the Si dimer rows shown in the STM line profile in Fig. 4(c) indicating these post-growth dimers may be composed of Sm. The spacing between ‘Sm dimers’ along a single row was measured as 0.76 nm. This is within experimental error of the measured periodicity and the accepted value of the periodicity,  $2a_{\text{Si}[110]}$ , of Si dimer rows. A ‘Sm dimer’ is observed to shift by  $0.5 \times 2a_{\text{Si}[110]}$  along a single row indicated by the arrow in Fig. 4(a). A schematic of a possible arrangement of Sm dimers on the Si(001) surface that is consistent with the experimental observations is shown in Fig. 4(d).

Sm dimers are oriented perpendicular to Si dimers forming a bond with the underlying Si atoms and arrange in rows with a spacing of  $1.5 \times 2a_{\text{Si}[110]}$  between rows. Dy atoms have been observed to form triple atomic strings, rather than dimers, on the Si(001) surface and a similar atomic arrangement has been proposed [10].

We have grown ordered arrays of  $\text{ErSi}_{2-x}$ ,  $\text{SmSi}_{2-x}$  and  $\text{DySi}_{2-x}$  nanowires oriented along Si[110] on vicinal substrates with a miscut of  $2.5^\circ$  toward [110]. In some cases, the nanowire length exceeds  $1 \mu\text{m}$  with wire widths on the order of a few nm. With low coverage of Sm, it appears that Sm dimers are present on the surface and arrange in rows oriented orthogonal to the underlying Si dimer rows. These dimers may serve as nuclei for nanowire growth and may account for the alignment of  $\text{RSi}_{2-x}$  on Si(001) vicinal substrates.

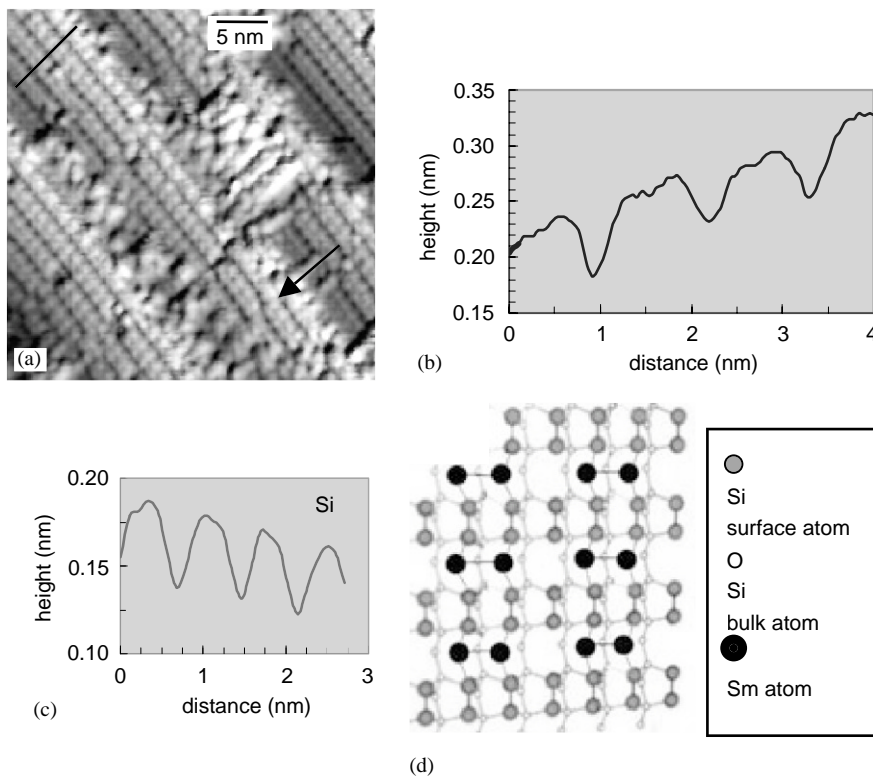


Fig. 4. (a) High-resolution STM image of the region in the square in Fig. 3(b). Arrow points to a region where dimers are offset by  $a_{\text{Si}[110]}$  in a single row. Line profiles taken at 2V across (b) the Sm dimer rows with a measured periodicity of approximately 1.2 nm where the profiled region is designated by a line in top left corner of (a), and (c) Si dimer rows with a periodicity of 0.8 nm, (d) a schematic of the possible arrangement of Sm dimer rows on the Si lattice.

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