

Perfect alignment of self-organized Ge islands on pre-grown Si stripe mesas

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Abstract. Self-organized Ge islands grown on patterned Si(001) substrates have been investigated. Selective epitaxial growth (SEG) of Si is carried out with gas-source molecular beam epitaxy to form Si stripe mesas followed by subsequent Ge island growth. Self-aligned Ge islands with regular spacing are formed on the $\langle 110 \rangle$ -oriented ridges of the Si mesas. The regular spacing is driven by the repulsive interaction between the neighbor islands through the substrates. A *mono*-modal distribution of the islands has been observed on the ridges of the Si mesas. The spatial confinement as well as the preferential nucleation is believed to be the mechanism of this alignment of the self-organized Ge islands.

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Self-organized islands have attracted considerable attention due to the fact that self-organization is able to realize nanostructures without using fine lithography and free of process-induced defects or damages, which are frequently seen in the samples defined by lithography and reactive ion etching. The potential device applications of self-organized nanostructures can be found in previous review papers [1]. The size distribution of self-organized islands has been extensively studied because the size uniformity of islands is a crucial concern for optoelectronic applications [2–6]. The spatial distribution of the islands is equally important in order to exploit computational and signal processing applications, for example, the quantum-dot cellular automata (QCA) [7, 8]. For some applications, only one-dimensional ordering of island arrays is needed. However, it is still a challenge to overcome the problem of random site distribution of the islands in order to accomplish ordered island arrays.

Facing the challenge, many efforts have been devoted in order to control the spatial distribution of self-organized Ge islands. These efforts include the growth of Ge islands on

the tilted substrates with the surface steps. The islands were somehow aligned along the step edges [9]. Relaxed template with misfit dislocations [10] and the stacking growth of multi-layer of islands [11, 12] were also utilized for controlling the location of self-organized islands. Even though some progresses have been made, the problem to control the ordering and position of the islands still remains.

Recently, the formation of one-dimensional arrays of Ge islands along the edges of the pre-grown Si stripe mesas has been reported [13]. In this alternating approach, by using SEG on the substrates with lithographic patterns, the stripe mesas were formed as a template for the subsequent Ge island growth. However, the islands also formed across the plateaus of the mesas, making the control of the island arrays difficult.

In this paper, we report the perfectly aligned self-organized Ge islands on the pre-grown Si stripe mesas to form one-dimensional island arrays after fully reducing the top plateaus of the stripe mesas. The average spacing between two islands increases with the decrease of the base width of the Si mesas. A *mono*-modal distribution of the islands is observed on the ridges of the Si mesas. The spatial confinement effect on the *mono*-modal distribution will be discussed.

1 Experiments

The substrates in this study were patterned Si(001), which were fabricated by conventional photo-lithography on thermally pre-grown silicon dioxide with a thickness of about 400 nm. The Si stripe windows were then opened along the $\langle 110 \rangle$ directions. Bare Si(001) substrates were used to accompany with the patterned samples in this study for comparison.

The patterned Si(001) substrates were cleaned by degreasing in organic solutions, and then cleaned by boiling in a mixture of $\text{NH}_4\text{OH} : \text{H}_2\text{O}_2 : \text{H}_2\text{O}$ (1 : 2 : 6 in volume), and finally transferred into a N_2 gas box and dipped in a diluted HF solution to form a hydrogen-terminated surface. The growth was carried out in a gas-source MBE system with a Si_2H_6 gas source and a Ge Knudsen-cell source. After thermal clean-

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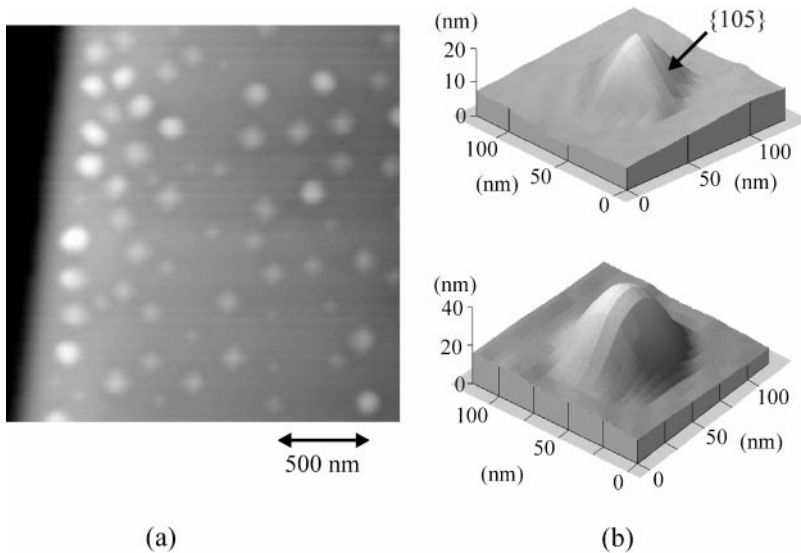


Fig. 1. **a** A two-dimensional AFM image of the self-organized Ge islands on a large Si mesa formed by SEG. A *bi*-modal size distribution of the islands can be seen. **b** The three-dimensional AFM images show two different modes of the Ge islands. The top is a smaller pyramidal island with four {105} facets, and the bottom is a larger dome-shaped island

ing at 890 °C, about 120 nm Si was selectively grown on the Si exposed windows at 660 °C with a growth rate of about 0.1 nm/s. The Si mesas with facets were thus formed. Details on the facet formation using the SEG process may be found in a previous publication [14].

After the Si growth, Ge was subsequently deposited at a growth temperature of 630 °C with a growth rate of about 0.01 nm/s. The Ge growth rate was stabilized by controlling the cell temperature within an error of ± 1 °C, and the rate was calibrated with Auger electron spectroscopy (AES) and atomic force microscopy (AFM) measurements. After the growth, the samples were taken out from the vacuum and inserted into a diluted HF solution to remove the silicon oxide on the surface for AFM study. The sample morphology and the Ge islands were then *ex situ* characterized with an AFM in a contact mode.

2 Results and discussions

Figure 1a presents an AFM image of the self-organized Ge islands on a large Si mesa. The areal density of the islands is about $1.6 \times 10^9 \text{ cm}^{-2}$ and the linear density along the edges is about $5.0 \times 10^4 \text{ cm}^{-1}$. The islands with smaller volume are pyramidal with four {105} facets, and the islands with larger volume have a dome shape (as shown in Fig. 1b). This is similar with the results on the bare Si(001) substrates. As normally seen in Ge/Si(001) system [15], a *bi*-modal size distribution of Ge islands could be seen on bare Si substrates. However, the difference is that the islands at the edges are bigger than those far from the edges, and the linear densities of the islands at the edges are larger than the areal density in the central region. Moreover, the islands tend to align with ordering along the edges rather than a random distribution in the other regions.

Due to the anisotropy of the growth rate in the SEG process, sidewall facets are formed and evolved from the dominance of the {113} facets at the initial stage of the SEG to the dominance of the {111} facets at larger Si thickness. Successive growth of Si reduces the lateral size of the top plateaus of the mesas leading to the full reduction in some smaller struc-

tures and the formation of the ridges. In this study, the {113} sidewall facets dominate the mesa sides at the Si thickness of about 120 nm.

Figure 2 (top) shows an AFM image of the self-organized Ge islands along an (110)-oriented Si stripe mesa with a base width of 0.7 μm . One-dimensional arrays of the Ge islands are formed on the ridges of the Si mesas. The formation of the ridges is due to the full reduction of the top plateaus of the Si mesas. No Ge islands on the {113} facets are observed. Figure 2 also shows the cross sections of the islands (middle) and the mesa (bottom). The island dimensions are about 90 nm wide and about 20 nm high, and the period of the Ge islands is about 110 nm. The average spacing between two islands increases with the decrease of the base width

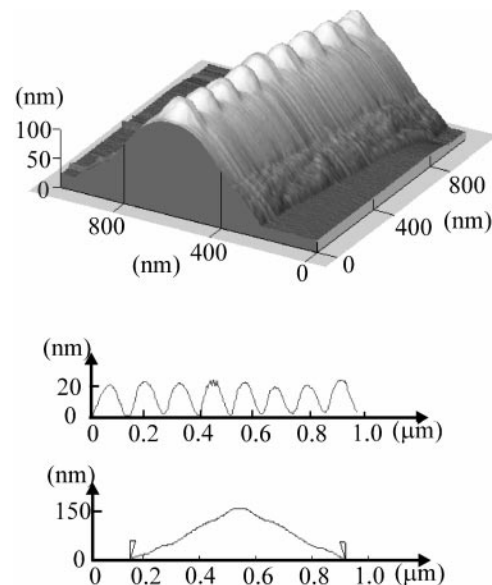


Fig. 2. A three-dimensional AFM image of the perfectly aligned and well-spaced Ge islands formed on the ridge of the Si mesa. The island size is about 90 nm. The *two curves* correspond to the cross sections of the island array (*middle*) and the Si mesa (*bottom*), respectively. The period of the island array is about 110 nm and the base width of the Si mesas is 0.7 μm

of the Si mesas. However, the size of the islands does not have a significant change. Only one row of the islands is observed on each Si stripe mesa with the base width varying from 0.5 μm to 1.0 μm . This indicates that it is very easy to control the island arrays on the stripe patterns in this width range.

For wider Si stripe patterns, the top plateaus of the Si mesas do not fully reduce (shown in Fig. 3). Therefore, on the Si plateaus (corresponding to the base width of the stripe mesas larger than 1.0 μm), the Ge islands are not only formed along the edges but also scattered in the central areas even though the edge sites are energetically preferential. This is due to the limit of the migration length of the Ge adatoms. We estimate the migration length of Ge adatoms at the temperature of 630 $^{\circ}\text{C}$ to be in the order of 0.3 μm . Compared with the island density on large mesas, the linear density of the single island array on the mesa ridges is about $9.0 \times 10^4 \text{ cm}^{-1}$, higher than that near the edges on large mesas ($5.0 \times 10^4 \text{ cm}^{-1}$). The islands in the central region of the mesas have a lower density than that near the edges. Moreover, the islands near the edges become larger as the width of the top plateau increases. This is the result of the migration of Ge from the central region of the plateau.

Ge islands are preferred to assemble close to each other on the mesa ridges. There are two plausible reasons for the island nucleation. From the viewpoint of energetics, the islands are most popular to sit at the sites with a minimum surface free energy. Previous cross-sectional TEM results [4, 9] show that Ge islands deform the underlying lattice to minimize the total free energy. Thus the convex curvature of the mesa ridges is beneficial to the formation of the Ge islands by partially relieving the strain energy since Ge has a larger lattice constant than the underlying Si. In addition, Ge adatoms have a suffi-

ciently long migration length to migrate to the favorable sites to form Ge islands and leave the other area free of Ge islands. The perfect alignment of the islands along the Si stripes is attributed to the preferential nucleation on the ridges and is assisted by the formation of the one-dimensional ridges. The regular spacing of the islands may be associated with the strain distribution underneath the islands. According to the theoretical prediction [16], there is a repulsive interaction between the islands through the deformation of the substrate lattice, which is caused by the strain field due to the island formation.

It is worth noting that a *mono*-mode distribution of the Ge islands rather than *bi*-modal distribution is observed on the ridges of the Si mesas. This means that all the islands are dome-shaped and have a close size distribution around 90 nm. A similar result on the high-index facets has been reported [17]. The *mono*-modal distribution of the islands on the one-dimensional ridges can be explained with the spatial confinement and the preferential nucleation. The Ge growth is in the Stranski–Krastanov growth mode. After a wetting layer, the Ge nucleates on the one-dimensional ridges due to the preferential nucleation. Meanwhile, in a SEG process, mass transfer from the sidewalls to the top plateau happens during the formation of the facets [18]. However, the migration along the one-dimensional ridges is limited due to the higher energy barrier to pass the islands. Therefore, Ge adatoms tend to migrate from both sidewalls leading to the formation of uniform islands, a *mono*-modal size distribution. This is different from the case, where the islands are randomly distributed on a plane and the migration can occur in a two-dimensional plane.

3 Conclusions

We have studied the self-organized Ge islands on the Si stripe mesas pre-grown by selective epitaxial growth. In particular, well-ordered one-dimensional Ge island arrays are formed on the ridges of the Si mesas with the base width varying from 0.5 μm to 1.0 μm . A *mono*-mode distribution of the islands has been observed on the ridges of the Si mesas. In comparison with larger plateaus, one-dimensional convex ridges are much easier to control the formation of the aligned islands. And the spatial confinement with the preferential nucleation results in a *mono*-modal size distribution. The one-dimensional ridge as a template may be an effective path to control self-organized island arrays or to realize a true sense of self-registration.

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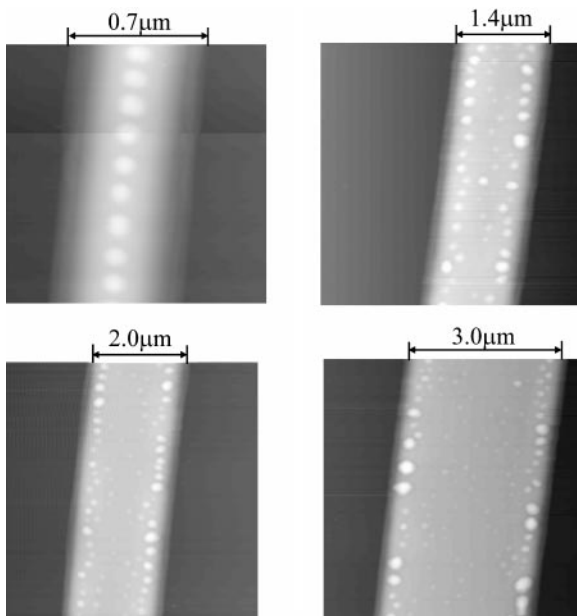


Fig. 3. Four AFM images show the dependence of the island distribution on the base width of the Si mesas. The base widths of the mesas are 0.7, 1.4, 2.0, and 3.0 μm , respectively. The transition from *mono*-modal to *bi*-modal size distribution of islands can be seen with the increase of the base width of the mesas

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