Shape change of SiGe islands with initial Si capping

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The morphologies of self-assembled Ge/Si(001) islands with initial Si capping at a temperature of 640 °C are investigated by atomic force microscopy. Before Si capping, the islands show a metastable dome shape with very good size uniformity. This dome shape changes to a pyramid shape with {103} facets at a Si capping thickness of 0.32 nm, and then changes to pyramid shapes with {104} and {105} facets at Si capping thicknesses of 0.42 and 0.64 nm, respectively. Noteworthy is that islands with one side retained their dome shape while the other three sides that changed to {103} facets are observed at a Si capping thickness of 0.18 nm. These observations indicate that island shape change with Si capping is a kinetic rather than thermodynamic process. The atomic processes associated with this island shape change are kinetically limited at a low temperature of 400 °C, and no significant change in size and shape of islands is observed when Si capping layers are deposited at this temperature. © *2005 American Institute of Physics.* [DOI: 10.1063/1.2137307]

Self-assembled SiGe islands[1,2] and rings[3] have been extensively investigated because of their potential applications and good compatibility with the current silicon technology.[4] When the islands or rings are put into actual applications in optoelectronic and microelectronic devices, it is necessary to bury islands or rings in Si; that is, to cap these nanostructures with Si layers. As the islands or rings are capped, the shape, size, and even strain and composition in the islands or rings will change, and these characteristic parameters for islands or rings determine their physical properties and relevant applications. So the knowledge of these parameters of islands or rings is important for the evaluation of their physical properties. On the other hand, the knowledge of these parameter changes with Si capping at different growth conditions is very helpful for a full understanding of island growth mechanism, and ring growth mechanism in particular. The latter has been obtained recently by capping islands partially.[3]

In this letter, the morphologies of islands at initial Si capping at a temperature of 640 °C are investigated by atomic force microscopy (AFM). Pyramid-shaped islands with {103} and {104} facets are observed when the dome-shaped islands are capped with a Si layer thickness of 0.32 and 0.42 nm, respectively. To our knowledge, no observation of pyramid-shaped islands bounded with {103} or {104} facets has been reported. Interestingly, islands with one side retained their dome shape while the other three sides that changed to {103} facets are observed at a Si capping thickness of 0.18 nm. The atomic processes associated with the shape change with Si capping are kinetically limited at a temperature of 400 °C, because the islands remained dome shaped after Si capping at this temperature.

The growth of islands was carried out in an ultrahigh-vacuum molecular-beam epitaxy (MBE) system (Riber Eva-32) with two electron-beam evaporators as Ge and Si sources. The base pressure of the system is better than 5×10^{-10} Torr. The substrate used was *p*-type Si (001) wafer with a resistivity of $1-10 \ \Omega$ cm. The substrates were chemi-

cally cleaned using the Shiraki method.[5] The protecting oxide on the substrate was desorbed at 1000 °C for 10 min in the growth chamber. The substrate temperature was then lowered to 640 °C, and a 50-nm-thick buffer layer was grown at a growth rate of 0.08 nm/s. A two-step growth method was adopted in island growth at a temperature of 640 °C in order to improve the uniformity of islands.[3,6] Uniform islands with a dome shape are obtained before Si capping. The Si capping layers of different thicknesses were deposited at a growth rate of 0.06 nm/s and at a temperature of 640 °C. To study the temperature effect on island morphology change with Si capping two samples were capped at a relatively low temperature of 400 °C. After the Si capping layer deposition, the substrate temperature was immediately cooled down to room temperature. The morphologies of the islands before and after Si capping are observed by atomic force microscopy (Solver P47-MDT) in contact mode in air.

Figure 1(a) shows the AFM image of islands grown at a temperature of 640 °C. These islands are clearly seen to have a dome shape, and they are believed to be metastable because both the size and shape of these islands are kept almost unchanged after *in situ* annealing for 5 min at the growth temperature of 640 °C as shown in Fig. 1(b). After a 0.32-nm-thick Si layer capping, the base size of the islands remains almost unchanged while the height of the islands decreases; meanwhile the shape of the islands changes from a dome to a pyramid as shown in Figs. 1(c) and 2(e). Figure 1(d) shows the cross-sectional profile of an island along [100], and the profile slope is obtained to be about 0.32, which is much closer to the slope 0.33 of the {103} facets. Therefore those islands are believed to be bounded with four {103} facets, and a small deviation from 0.33 may be caused by the AFM tip effect. The {103} facets are further verified by the two-dimensional statistical histogram of the orientation of the facets,[7] as shown in Fig. 1(e). The partial derivatives of height to transverse axis have four typical values which correspond to four {103} facets. Stoffel *et al.* have reported new {117} facets of islands which coexisted with {113} facets,[8] however, to our knowledge, this is the first observation of pyramid islands bounded with {103} facets

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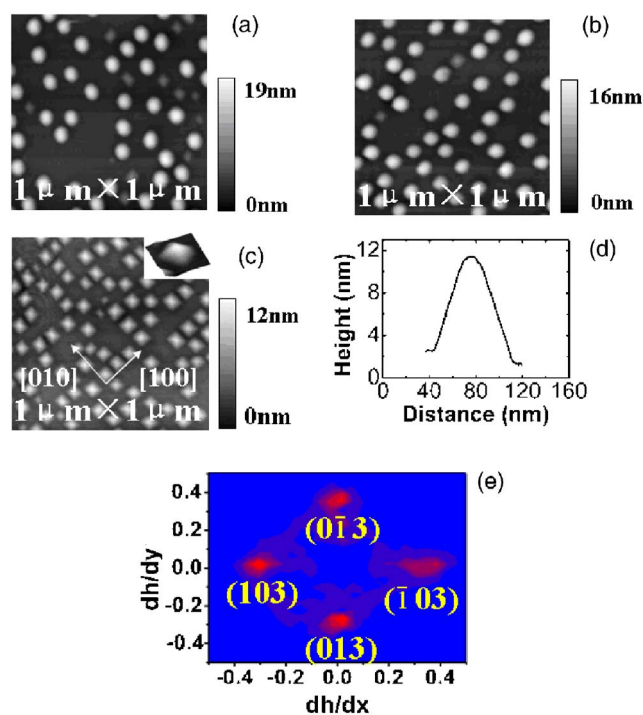[a)]Author to whom correspondence should be addressed; electronic mail: zmjiang@fudan.ac.cn

FIG. 1. (Color online) AFM images (1.0×1.0 μm) of SiGe islands: (a) as grown, (b) after *in situ* annealing for 5 min at 640 °C, (c) after capping with a 0.32-nm-thick Si layer at 640 °C. (d) The cross-sectional profile of a capped island in (c) along [100]. (e) A two-dimensional statistical histogram of the orientation of the facets as shown in Fig. 3(c).

and these {103}-faceted-pyramid islands are only observed during initial Si capping. When the Si capping layer thickness increases to 0.64 nm, the island shape changes to a {105}-faceted pyramid as observed previously,[9,10] with the slopes of facets being between 0.19 and 0.20.

Generally speaking, with Si capping the island shape changes from a dome to a pyramid, followed by an inclination of pyramid facets decreasing with facets changing from {103} to {104}, and then to {105}, as shown in Fig. 2. The
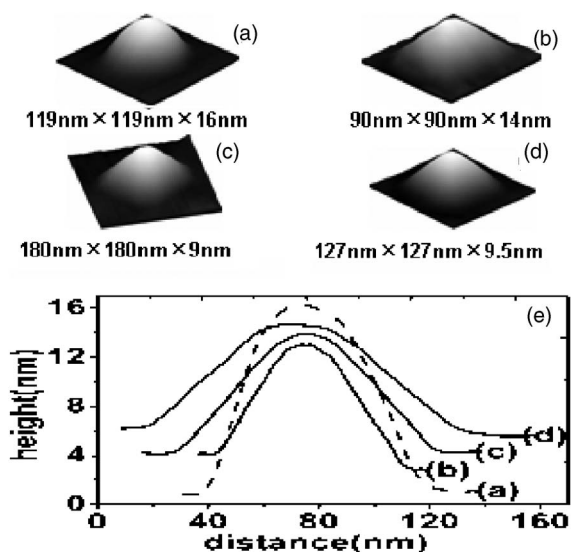

FIG. 2. AFM images of islands (a) before Si capping and after capping with a Si layer thickness of (b) 0.32, (c) 0.42, and (d) 0.64 nm at 640 °C. Note that the different scan scales are indicated for each image. (e) The corresponding cross-sectional profiles along [100]; the curves are shifted vertically in order to clearly show the different facet slopes.
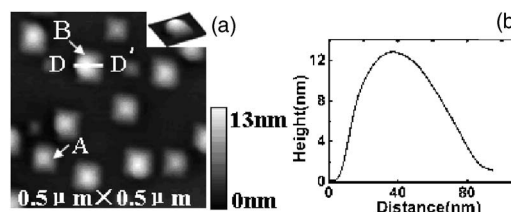

FIG. 3. (a) AFM images (0.5×0.5 μm) of SiGe islands capped with a 0.18-nm-thick Si layer at 640 °C; the inset is a three-dimensional AFM image of an island with the transition shape. (b) The cross-sectional profile of an island as denoted by *B* in Fig. 3(a) along the *D-D'* line.

islands become more and more dwarf with Si capping. This implies that the morphology change of islands with Si capping is a kinetic rather than a thermodynamic process.[9]

Interestingly, when islands are capped with a 0.18-nm-thick Si layer, which is less than the thickness (0.32 nm) for a complete shape transformation for all islands from a dome to a pyramid bounded by {103} facets, some island's shapes change to a pyramid with {103} facet as denoted by *A* in Fig. 3(a), while some islands show a shape between a dome and a pyramid with one side retaining a dome shape and the other three sides changing to {103} facets as denoted by *B* in Fig. 3(a). Figure 3(b) is the cross-sectional profile of a transition island (*B*) along the *D-D'* line, showing clearly a steep slope at the left-hand side for a dome shape and a less steep slope of {103} facet at the right-hand side. These observations further show that the island shape change with Si capping undergoes a kinetic process and this kinetic process is not fast, with a time scale of tens of seconds or more at the temperature of 640 °C. If this kinetic process with a time scale is less than a few seconds, it will be very hard to observe those islands with transition shape at our conventional MBE growth condition.

This kinetic process for island shape change with Si capping is believed to be driven by the strain relaxation. The atomic processes in this kinetics may be associated with Ge atoms diffusing away from island to wetting layer, Ge atom surface segregating from the island's inner part to the island's surface, and the arriving capping Si atoms incorporating into islands. All those processes are favorable for the strain relaxation of islands with Si capping. As shown in Fig. 4, at a 0.32-nm-thick Si layer capping, the island volume becomes smaller and the average Ge composition in the island, which is estimated by x-ray diffraction, becomes smaller too. It indicates that certain Ge atoms that were previously in the island diffuse away, reducing the strain in the island. At the same time, Ge surface segregation will take place at this temperature in order to compensate Ge atoms on
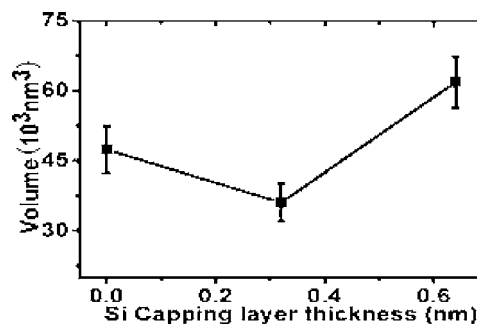

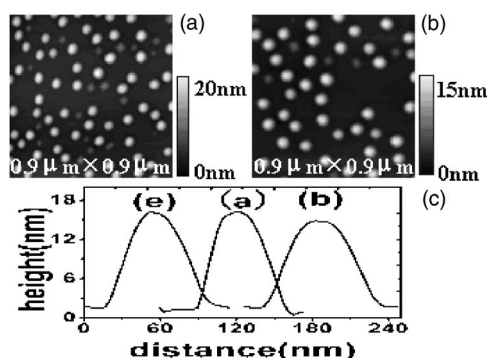FIG. 4. The island volume as a function of Si capping layer thickness.

FIG. 5. AFM images $(0.9 \times 0.9 \ \mu m)$ of SiGe islands after capping at a temperature of 400 °C with a Si layer thickness of (a) 0.32 and (b) 0.64 nm. (c) The cross-sectional profiles of an island capped at 400 °C with a Si layer thickness of [curve (e)] 0, [curve (a)] 0.32, and [curve (b)] 0.64 nm.

the island surface, thereby reducing the average Ge composition and strain as well in the island. At a 0.64-nm-thick Si layer capping, the volumes of islands became much larger compared with islands at a 0.32-nm-thick Si layer capping, as shown in Fig. 4, which suggests that a large amount of Si atoms were added to the islands. Adding Si atoms into the islands is also favorable for the strain relaxation, in that it reduces the total energy of the islands as observed by Denker *et al.*[11]

To study the temperature dependence of those atomic kinetic processes, Si capping layers were deposited at different temperatures. Two samples were capped at a low temperature of 400 °C. As shown in Fig. 5(c), although the height of the islands decreased slightly, the shape of the islands was well preserved, as observed by Stoffel *et al.* after Si capping below 400 °C. (Ref. 8). It means that all the atomic processes for strain relaxation of the island are kinetically limited at this temperature, resulting in no significant change in island shape and size. As the deposition temperature increases to 500 °C, a significant shape change of the islands was observed after Si capping. Therefore, if one needs to preserve the island shape and size with Si capping or to bury islands with the shape and size preserved, the deposition temperature for the Si capping layer should not be higher than 400 °C in order to kinetically hinder the atomic processes responsible for island shape and size change. It may also be possible to bury islands without shape and size changes at a much higher Si deposition rate, which makes the atomic processes associated with island shape and size change relatively slower in comparison with the high Si deposition rate. As we know, low-temperature growth will result in defects, especially point defects, in the grown layer. One approach to solve the problem is to bury islands at a low temperature plus a postgrowth annealing at a higher temperature, which will eliminate most point defects formed at low-temperature growth. The atomic processes responsible for island shape and size change are all surface processes which will be kinetically limited during Si capping at a low temperature. After a thick Si layer capping, the only one atomic process to cause the buried island shape and size change during a postgrowth annealing is atomic interdiffusion, which will take place significantly at a temperature much higher than 400 °C.

Finally, we point out that although the strain relaxation is the driving force for island shape change during the Si capping; that is, the strain relaxation plays a key role for island shape change during Si capping, the surface energies of facets may also play a role in the island shape change. This may be the reason why only those pyramid-shaped islands with particular low-index facets, such as {103}, {104}, and {105}, are observed.

In summary, the shape change of self-organizing islands on Si (001) at initial Si capping is investigated. Islands changed shape from a dome to a pyramid bounded with {103}, {104}, and {105} facets after Si capping at 640 °C at a capping layer thickness of 0.32, 0.42, and 0.64 nm, respectively. The observation of shape transformation indicates island shape change is a kinetic process with a time scale of more than tens of seconds at 640 °C, which is suggested to be driven by strain relaxation of the island and associated with both Ge and Si atomic surface diffusion and Ge atomic surface segregation. Those atomic surface processes responsible for island shape and size change with Si capping are totally kinetically limited at temperatures below 400 °C.

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