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Citation: Journal of Applied Physics 112, 126101 (2012); doi: 10.1063/1.4770408

View online: http://dx.doi.org/10.1063/1.4770408

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A transition of three to two dimensional Si growth on Ge (100) substrate

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(Received 23 October 2012; accepted 26 November 2012; published online 21 December 2012)

For the initial growth of Si on Ge, three-dimensional Si quantum dots grown on the Ge surface were observed. With increasing Si thickness, the Si growth changes from three-dimensional to two-dimensional growth mode and the dots disappear gradually. Finally, the surface is smooth with the roughness of 0.26 nm, similar to the original Ge substrate, when 15 nm Si is deposited. More Ge segregation on the wetting layer leads to more open sites to increase the subsequent Si growth rate on the wetting layer than on the Si dots. The in-plane x-ray diffraction by synchrotron radiation is used to observe the evolution of tensile strain in the Si layer grown on Ge (100) substrate. © 2012 American Institute of Physics. [http://dx.doi.org/10.1063/1.4770408]

SiGe quantum wells (QWs)^{1,2} and quantum dots (QDs)^{3,4} have drawn much attention in the applications of nanoelectronics and optoelectronics. The three-dimensional, a growth mode (Stranski-Krastanov, SK) is well-known to dominate the Ge epitaxial growth on Si.5,6 A few monolayer of Si directly grown on Ge has been reported to passivate Ge channels of metal-oxide-semiconductor field effect transistor (MOSFET).^{7,8} A doped epi-Si layer was reported to eliminate Fermi level pinning and to reduce the contact resistivity. However, there are limited reports on the growth mode of Si on Ge. The dot growth of 4-20-monolayer Si on Ge (001) by molecular beam epitaxy (MBE) was studied over a wide range of growth temperatures. Under tensile strain, the Si dots with SK growth mode were analyzed. 10 However, the further growth can lead to Ge segregation on the surface. The Ge segregation has been found in MBE and ultra-high vacuum chemical vapor deposition (UHV/CVD) system due to the hydrogen desorption from the surface¹¹ and it can happen even at the temperature lower than 300 °C. 12 The open sites created by the Ge segregation on the Si surface are responsible for the growth mode transition from the traditional threedimensional mode. The growth mode transition of Si on Ge is observed by the atomic force microscopy (AFM) and the cross-sectional transmission electron microscopy (TEM).

All the samples were grown by the UHV/CVD system at 550 °C. The base pressure was $\sim 10^{-9}$ torr. Pure silane (SiH₄) at a fixed 100 sccm flow was used for Si growth. The Si is directly grown on Ge without the buffer layer. The Si dots grown at 550°C are shown in Fig. 1(a) with the dot density of $\sim 7 \times 10^8 \, \mathrm{cm}^{-2}$ and the surface root-mean-square (RMS) roughness of \sim 1.21 nm. The much lower density as compared to the Ge dots on Si ($\sim 10^{10} \, \text{cm}^{-2}$) probably due to the impedance of three-dimensional dot growth by the tensile strain. 13,14 The aspect ratios of Si dots on Ge are from ~ 0.05 to ~ 0.1 , which are smaller than the Ge dots on Si (0.13–0.17). ¹⁴ The cross sectional TEM image of the Si dot with the aspect ratio of ~ 0.05 is shown in Fig. 1(b). The wetting layer of the Si dot is \sim 5 nm, which is thicker than that of the Ge dot on Si (\sim 1 nm). The thicker wetting layer of Si dot on Ge was also reported in Ref. 10. The observed thicker wetting is probably due to the tensile strain.¹³ It is evident that the SK mode growth is still valid for the tensile strained Si growth on Ge (001). 10

However, while the Si thickness increases, the surface morphology changes. No dots were observed on the surface with the Si thickness of $\sim 11 \,\mathrm{nm}$ (Fig. 2(c)). Instead, the smooth surfaces (RMS roughness ~0.91 nm) with scattered ring-like structures were observed on the surface (Fig. 2(a)). The density of the ring-like structure is $\sim 2 \times 10^7 \, \mathrm{cm}^{-2}$. The Fig. 2(b) shows the 3D AFM image of the ring-like structure. The ring average diameter and depth is \sim 131 nm and \sim 0.9 nm, respectively. For Ge growth on Si, the ring could be due to the SiO₂ particles from other's work¹⁵ or surface diffusion of adatoms to relatively strain-free regions from our early work. ¹⁶ For Si growth on Ge, since the strain is almost relaxed at Si dot facet on Ge substrate, ¹⁷ the Si adatoms can diffuse to relatively strain-free facet regions and aggregate on the facet of the Si dot to form the ring-like structure in this work. Moreover, no oxide at Si/Ge interface was detected by the energy dispersive x-ray spectroscopy (EDS). The three-dimensional to two-dimensional transition of Si growth would not be expected if there was some oxide on the initial Ge surface. In the TEM image (Fig. 2(c)), it is found that the dots disappeared after the growth of \sim 11 nm Si film. Due to the small aspect ratio (\sim 0.007) of the ring-like structure, it is difficult to observe the ring-like structure on the cross sectional TEM image. Note that some dislocations were observed in the Si film which can relax tensile strain.

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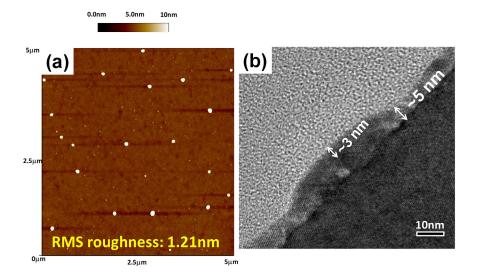


FIG. 1. (a) The AFM image of Si dots on Ge with surface root-mean-square roughness \sim 1.21 nm. (b) The cross-sectional TEM image of a Si dot with the wetting layer of \sim 5 nm and the dot height of \sim 3 nm.

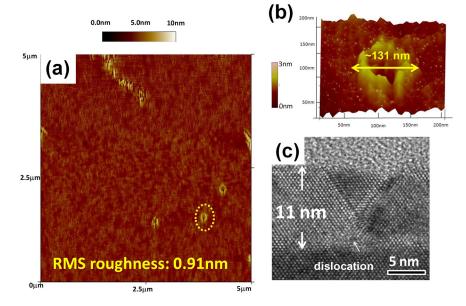


FIG. 2. (a) The AFM image of the \sim 11 nm Si film with ring-like structures on the surface. (b) The 3D AFM morphology of the ring-like structure. The average diameter and depth is \sim 131 nm and \sim 0.9 nm, respectively. (c) The cross-sectional TEM image of the \sim 11 nm Si on Ge. Note the dislocation appears to relax strain.

Growth rate enhancement on the wetting layer plays a crucial role in the growth mode transition for Si growth on Ge. The Ge can segregate on Si surface with the activation energy $\sim 1.4 \,\mathrm{eV}$. The Ge segregation in our samples is observed by the EDS measurement. For the Si dot grown on Ge, the Ge content at the wetting layer surface is \sim 37%, which is much higher than that at the dot (\sim 10%) (Fig. 3(a)). Since the desorption energy of hydrogen from Ge (100) surface (~1.51 eV) is lower than that from Si (100) surface $(\sim 2.05 \,\mathrm{eV})$, the hydrogen desorption increases due to the increasing Ge coverage on the surface. 19 Since there is more Ge segregation on the wetting layer (\sim 5 nm) for Si growth on Ge surface after the three-dimensional dot growth, more open sites yield a higher Si growth rate on the Si wetting layer than on the Si dots.²⁰ Higher subsequent Si growth rate at the wetting layer than the Si dots leads to the transition of three-dimensional Si dot growth to the two-dimensional Si film growth (Fig. 3(b)).

After \sim 15 nm growth of Si on Ge (Fig. 4), neither Si dots nor ring-like structures were observed on the surface. The surface RMS roughness is only about \sim 0.26 nm, which

is similar to the bulk Ge substrate (\sim 0.25 nm). From the EDS measurement (Fig. 4), the Ge content is \sim 47% near the bottom of "Si film" and gradually decreases to \sim 2% near the top due to Ge diffusion into Si. With the assistance of the enhanced growth rate at the initial Si wetting layer, the transition from three-dimensional to two-dimensional growth mode was observed for Si growth on Ge. For even thicker Si, less Ge content near the top is expected.

The evolution of strain in Si on Ge, which is determined by the lateral lattice constant, was analyzed by the in-plane x-ray diffraction (XRD) using synchrotron radiation source. The XRD in-plane radial scans across Si (400) and Ge (400) peaks for the samples with Si dots and 15 nm Si on Ge are shown in Fig. 5. The decrease of lateral lattice parameter, as revealed by the positive shift of $\sim 0.5^{\circ}$ from the Si dot sample to the 15 nm Si film sample, is attributed to the relaxation of lateral tensile strain. Note that the Si dots have the lateral tensile strain of $\sim 0.34\%$. With the increasing Si thickness, the strain relaxation becomes significant. The 15 nm Si on Ge is almost relaxed. The dislocation in the 15 nm Si film (Fig. 4) is responsible for the tensile strain relaxation.

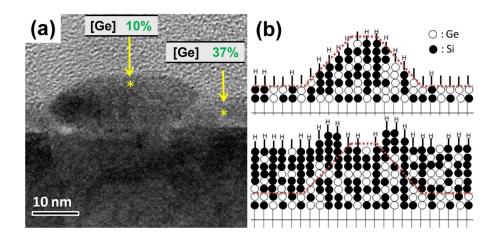


FIG. 3. (a) The EDS measurement for a Si dot on Ge. (b) The growth schematic of Ge segregation effects of Si grown on Ge. Higher growth rate due to the more open sites on the wetting layer than on the dot leads to the smooth surface.

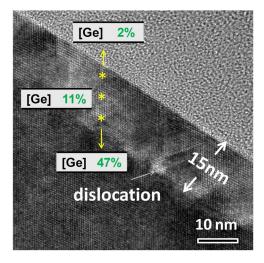


FIG. 4. The cross-sectional TEM images with Ge content by EDS measurement.

In summary, the transition of growth mode from threedimensional to two-dimensional for Si growth on Ge has been observed for the first time. The enhanced Si growth rate due to the Ge segregation on the wetting layer leads to such transition. Smooth Si growth directly on Ge can be used for the applications of novel nanoelectronics and optoelectronics.

The support of National Science Council of Taiwan, R.O.C. (contract Nos. 100-2221-E-002-181-MY3 and 100-2120-M-002-012), the Military of Education (5 yr 50 B program), and Applied Materials are highly appreciated.

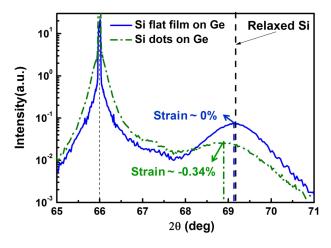


FIG. 5. The (400) XRD in-plane radial scans of Si dots and 15 nm Si on Ge. Note the tensile strain is almost relaxed for 15 nm Si on Ge.

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