Critical thickness of strained Si$_{1-x}$Ge$_x$ on Ge(111) and Ge-on-Si(111)

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Critical thicknesses ($t_c$) of Ge-rich strained Si$_{1-x}$Ge$_x$ layers grown on various Ge substrates are precisely determined experimentally, and $t_c$ is revealed to strongly depend on the substrate conditions. We find that $t_c$ of Si$_{0.24}$Ge$_{0.76}$ on Ge-on-Si(111) is much lower than that on the Ge(111) substrate for $x > 0.75$ while, for $x < 0.75$, $t_c$ becomes equivalent between both substrates, origins of which can be discussed in terms of dislocation nucleation and surface ridge formation. This study provides critical design parameters for strained SiGe(111) based devices, such as high-mobility channels and spintronic devices on a Si platform.

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[Fig. 1(c)], the number of the ridges increases and the relaxation ratio also increases to 3%, indicating that this thickness exceeds $t_c$. From the observation of other samples, it was found that the density of the ridges gradually increases as the layer thickness increases. Figure 1(d) shows an AFM image of the selected region of the LM image in Fig. 1(c). The line-shaped ridge is very clearly seen and its height and width are estimated to be around 10 nm and 1–2 μm, respectively. It is also found that outside of the ridge, the SiGe surface is very flat. Values of mean surface roughness (Ra) obtained by AFM are 0.07–0.10 nm for the 50 nm thick layer and 0.1–0.3 nm for the 130 and 180 nm thick layers.

Strain states in and out of the ridge regions are investigated by micro Raman measurements. Since the width of the ridge is 1–2 μm, the laser beam can be focused within the ridge and spectrum only from the ridge region can be obtained. Figure 2 shows Raman spectra in and out of the ridge for 180 nm thick Si$_{0.24}$Ge$_{0.76}$ on Ge(111). The Ge-Ge, Si-Ge and Si-Si phonon mode peaks in the ridge are observed to shift to higher wavenumbers from those out of the ridge. Here, peak shifts $\Delta\omega_{\text{Ge-Ge}}$ and $\Delta\omega_{\text{Ge-Si}}$ are defined as differences in Raman peak values between in and out-of ridge regions for Ge-Ge and Si-Ge phonon modes, respectively, as shown in Fig. 2. In general, such phonon mode peaks shift due to the modification of strain and/or Ge contents in SiGe layer.\(^29,30\)

On the other hand, it is expected that the Ge-Ge and Si-Ge mode peaks shift to higher wavenumbers whereas the Si-Si mode peak shifts to lower wavenumbers with increasing Ge contents in a SiGe layer. Therefore, considering the observation of the peak shifts (Fig. 2), it can be concluded that the tensile strain in the ridge region is partially relaxed and the Ge content modification is negligible. A relaxation ratio in the ridge region is estimated to be approximately 60% from the obtained $\Delta\omega_{\text{Ge-Ge}}$ (2.3 cm$^{-1}$). Inset shows $\Delta\omega_{\text{Ge-Ge}}$ and $\Delta\omega_{\text{Ge-Si}}$ as a function of the SiGe thickness. As the thickness increases, the peak shifts also increase, which means the strain relaxation proceeds with the thickness locally in the ridge. On the other hand, the relaxation hardly takes place on the ridge-free areas, resulting in averaged wide-area relaxation ratios as low as 3% obtained by XRD in nm scale.

An origin of the ridge formation can be considered as follows. First, due to the strain energy accommodated in the strained SiGe film, misfit dislocations are nucleated at an interface between the SiGe and Ge and glide through equivalent (111) slip planes. The tensile strain in the SiGe is locally relieved along the dislocations, leading to laterally inhomogeneous strain distribution. Due to this the growth rate of the SiGe is locally modified and the SiGe growth thickness is enlarged around the dislocations, forming the surface ridges. Similarly to the dislocations, the directions of the ridges correspond to intersections of the equivalent (111) planes and the surface (111) plane as seen in Fig. 1. From the derived relaxation ratios (~50%), a number of dislocations are speculated to be generated and accumulated after gliding within the ridge region, and detailed observation of the dislocations is underway. These line-shaped ridges were also observed for Si$_{1-x}$Ge$_x$ layers grown on the Ge-on-Si(111) and Ge(100) substrates with various thicknesses and compositions whereas the conditions are quite different depending on the substrates, which will be discussed below.

Next we investigated changes in the surface morphologies after annealing. It was confirmed by LM measurements (not shown here) that the distribution as well as the density of the ridges appearing before annealing remain unchanged after annealing. Figures 3(a) and 3(b) show AFM images in ridge-free regions.
free areas of the 130 nm thick Si$_{0.25}$Ge$_{0.75}$ on the Ge(111) substrate before and after annealing, respectively. While the surface has no roughness before annealing, a number of trenches are generated after annealing. Their directions are along [10−1], [−110] and [0−11], that is, the intersections of equivalent (111) planes and the surface, which is the same as the ridges observed in Fig. 1. High density trenches with those directions are clearly forming partial triangle shapes. These results imply that the trenches are formed due to misfit dislocation gliding towards the surface during the annealing. Strain relaxation ratio obtained by XRD from the wide-area significantly increases from 0 to 29% after annealing. By characterizations for other SiGe samples, it was confirmed that the density of the dislocation-related trenches increases as the layer thickness increases, leading to the larger relaxation ratios. It is noted that, unlike the SiGe layers on Ge(111) substrates, high density ridges appear for thinner SiGe layers on Ge-on-Si(111), which means $t_c$ of SiGe on Ge-on-Si is lower.

Figure 4 summarize results of all SiGe samples fabricated in this study, i.e. various thickness Si$_{1−x}$Ge$_x$ layers on the Ge (111), Ge-on-Si(111) and Ge(100) substrates in the top, middle and bottom graphs, respectively. One plot corresponds to one sample in each graph, where $x$ and $y$ axes represent Ge concentrations in SiGe and the SiGe thickness, respectively. Red square plots represent samples which were partially relaxed after the growth. Green triangle plots represent samples which were fully strained after the growth but partially relaxed after annealing. Blue circle plots represent samples which were fully strained even after annealing. For these plots, XRD results were used for judging whether the SiGe is fully strained or partially relaxed. In contrast, from observations of surface morphologies, filled plots are used for samples which exhibited a very flat surface without any ridges after the growth while open plots correspond to samples where the surface ridges clearly appeared before annealing. Boundaries of blue and green plots represent equilibrium $t_c$ curves while those of green and red do meta-stable $t_c$ curves as shown with dashed lines. Also, we can write other curves (solid line) at boundaries of open and filled plots, which mean $t_c$ for growth of ridge-free surfaces. It is clearly seen in those three graphs that $t_c$ rapidly decreases with the decrease in Ge contents, that is, the increase in the tensile strain. This behavior is almost the same as reports on SiGe/Si(100) system and theoretically predictable. However, it is remarkable that the values of $t_c$ depends strongly on the Ge substrates, which has not been reported in detail so far.

It is noticeable that $t_c$ of Si$_{1−x}$Ge$_x$ layers on the Ge-on-Si (111) is much lower than that on the Ge(111) substrate especially Ge contents higher than 75%. For example, at the Ge content of 90% $t_c$ is 110 and 260 nm for Si$_{0.1}$Ge$_{0.9}$ layers on the Ge-on-Si(111) and Ge(111), respectively. This difference is presumably because threading dislocations in the Ge epilayer on Si work as sources for misfit dislocation nucleation and facilitate the strain relaxation of Si$_{1−x}$Ge$_x$ layers on the Ge-on-Si(111) substrate. Additionally, the Ge layer grown on Si(111) has 0.2% tensile strain due to differences of thermal expansion coefficients between Ge and Si. This tensile strain in Ge-on-Si is added to the tensile strain of overgrown SiGe layers, leading to the higher probability of the dislocation nucleation and resultantly lower $t_c$. By contrast, for Ge concentrations lower than 75%, $t_c$ is equivalent between Ge(111) and Ge-on-Si(111) substrates. For example, for Si$_{0.3}$Ge$_{0.7}$ layers both on the Ge-on-Si(111) and Ge(111), $t_c$ determined by the ridge formation, which is slightly lower than equilibrium $t_c$ determined by XRD, is about 35 nm. In this Ge content range, the above mentioned effects do not play roles for relaxation for both structures. In other words, the Ge-on-Si fabricated here has sufficiently high quality for the strained SiGe growth with several tens nm, which is thick enough for device channel formation. On the other hand, $t_c$ of Si$_{1−x}$Ge$_x$ layers on Ge(100) is higher than that on Ge(111) substrates. This is presumably attributable to different dislocation generation mechanisms. For SiGe/Ge(111), the hetero-interface is (111) plane and can become the slip plane for dislocations. Therefore, nucleation of dislocations in SiGe/Ge(111) is much more likely than that in SiGe/Ge (100), resulting in the lower $t_c$ for SiGe/Ge(111). It is also noticeable that the solid curves ($t_c$ for ridge-free surface) are close to but do not correspond to equilibrium $t_c$ (dashed lines). Since the strained SiGe with a ridged surface cannot be employed for device channels, it can be said that

![Figure 4](Color online) Summary of results of all SiGe samples fabricated in graphs of SiGe thickness versus Ge concentrations in SiGe for (a) SiGe/Ge(111), (b) SiGe/Ge-on-Si(111) and (c) SiGe/Ge(100) substrates. See the text for each plot and curve.
acceptable conditions are below both the solid and dashed curves, which have firstly been indicated.

In summary, experimental critical thickness ($t_c$) of strained Si$_{1-x}$Ge$_x$ layers grown on Ge-on-Si(111) and Ge(111) substrates were studied. To determine $t_c$, initial stages of strain relaxation of the Si$_{1-x}$Ge$_x$ layers were investigated in detail, where strain states together with surface morphologies were systematically evaluated by XRD, micro-Raman, laser microscope and atomic force microscope. As a result, experimental critical thickness ($t_c$) of strained Si$_{1-x}$Ge$_x$/Ge-on-Si(111) is much lower than that of Si$_{1-x}$Ge$_x$/Ge for the higher Ge concentrations in SiGe. This different behavior of $t_c$ found in this comparative study has to be considered carefully for applications of strained Si/Ge heterostructures on Ge-on-Si to various devices.

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