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Suppression of structural imperfection in strained Si by utilizing SiGe bulk substrate

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We attempted to utilize homemade SiGe bulk crystal as a substrate for epitaxy of strain-controlled heterostructures. X-ray reciprocal space mapping clarified that the growth of a Si thin film on a SiGe bulk substrate leads to reduction in the orientation fluctuation compared with that on a SiGe virtual substrate. Furthermore, analysis of Raman spectra revealed a dramatic decrease of the strain fluctuation in the strained Si film on the SiGe bulk substrate. These results suggest that the SiGe bulk crystal can be utilized as a substrate for various strain-controlled heterostructures for fundamental studies as well as improvement of device performance. © *2006 American Institute of Physics*. [DOI: 10.1063/1.2208928]

The ability to control the strain in SiGe thin film has led to a renewed interest in the group-IV heterostructures.[1] Extraordinarily high electron mobilities[2] and their limiting mechanisms[3] have been reported using strained Si channel modulation doped structures. A pair of quantum wells with tensilely strained Si(C) and compressively strained SiGe layers has been reported to show intense photoluminescence with enhanced no-phonon transition.[4,5] Establishment of fabrication process of high-quality strain-relaxed SiGe on Si has been regarded as a key issue for tailoring the strain-controlled band engineering in group-IV heterostructures since relaxed SiGe can be used as a "virtual" substrate with a larger lattice constant than that of Si. Although several methods have been attempted to obtain SiGe virtual substrates,[6–11] misfit dislocations are necessarily introduced to relax the strain in SiGe owing to the lattice mismatch between SiGe and Si, leading to structural imperfection such as fluctuation in the orientation and the strain.[12] The overgrown Si film will succeed the structural imperfection of the virtual substrate, which would deteriorate the transport and optical properties. In order to have access to the intrinsic properties of strained Si, the structural imperfection of the substrate must be somehow suppressed.

A straightforward approach is to utilize SiGe bulk crystal as a substrate for epitaxial growth of strained Si. However, it is difficult to realize SiGe bulk crystal with uniform composition as can be understood by the phase diagram.[13] In the melt growth under near equilibrium conditions, the composition in solid SiGe is determined by the temperature at the growth interface. Due to the large difference in the melting point of Si and Ge, the solidus line of the phase diagram is strongly dependent on the temperature. Therefore, the precise control of the temperature at the growth interface is required. Furthermore, crystal growth results in the depletion of Si in the melt due to the deviation of the segregation coefficient from unity. To overcome these difficulties, several methods have been attempted including *in situ* monitoring of the temperature at the interface[14,15] and its feedback control,[16] realization of the steady state with the effective segregation coefficient of unity,[17–19] and so on.

In this letter, we report on our attempt to utilize homemade Si-rich SiGe bulk crystal as a substrate for strained Si thin film. Epitaxial growth of Si thin film was carried out both on a SiGe bulk substrate and on a conventional SiGe virtual substrate. By x-ray reciprocal space mapping, the orientation fluctuation in the strained Si layer was revealed to be suppressed by exploiting SiGe bulk substrate. In addition, analysis of microscopic Raman spectra clarified that the strain fluctuation in the strained Si layer can be reduced by growing on the SiGe bulk substrate.

The growth of the SiGe bulk crystal was started by setting a 15-mm-long Si(100) seed crystal and a 10-mm-long Ge crystal with a diameter of 15 mm in a crucible made of quartz and carbon. The crucible was set in a high temperature furnace, and a part of the Si crystal and the Ge crystal are melted. Since the Si solute elements diffuse into the Ge melt, SiGe binary melt is formed. The SiGe bulk crystal was then grown in an Ar atmosphere by moving the crucible toward lower temperature zone at a constant rate. An appropriate choice in the pulling rate is considered to lead to a constant interface temperature, leading to the uniform Ge composition in the grown crystal.[18] This process is depicted in Fig. 1. The Ge composition of the grown crystal was around 0.15–0.20, and showed gradual increase along the growth direction. The SiGe bulk crystal was sliced perpendicular to the growth direction, and the mirror surface was obtained by chemomechanical polishing treatment after mechanical polishing. Epitaxial growth on the $Si_{0.85}Ge_{0.15}$ substrate was carried out in a gas-source molecular beam epitaxy (MBE) system (AirWater VCE S2020) using disilane and germane as source gases. Following the growth of a SiGe buffer layer, a 50 nm Si thin film was grown at the growth temperature of 560 °C. As a control sample, strained Si film was also grown on a SiGe virtual substrate fabricated by epitaxial growth of SiGe on Si(100).

Figure 2 compares results of x-ray diffraction of $2\theta/\omega$ scan around {004} reflection of strained Si (a) on the SiGe virtual substrate and (b) on the SiGe bulk substrate. It is seen that the SiGe {004} reflection consists of one broad peak in Fig. 2(a), while that in Fig. 2(b) contains two sharp peaks. The appearance of two peaks originates from unintentional mismatch in the Ge composition between the substrate and

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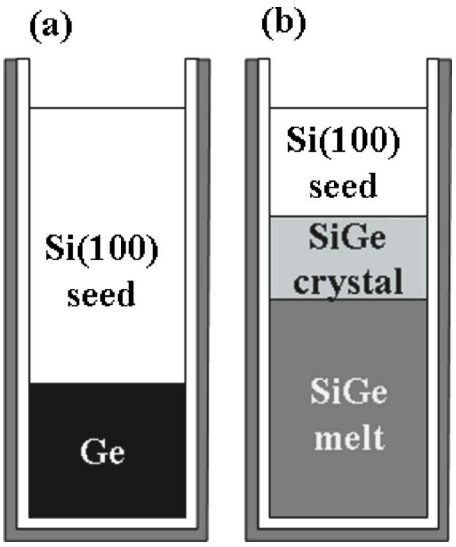

FIG. 1. (Color online) Illustration of (a) initial setting of raw materials in a double crucible and (b) the situation during growth.

the buffer layer. Importantly, sharp peaks observed in Fig. 2(b) reflects the fact that the SiGe bulk substrate and the SiGe buffer layer are of high structural quality. At the higher diffraction angle of the SiGe peak, a peak can be clearly seen, which can be assigned as coming from the strained Si layer on the SiGe bulk substrate.

Figure 3 shows x-ray reciprocal space mapping around {224} of strained Si (a) on the SiGe virtual substrate and (b) on the SiGe bulk substrate. The horizontal and the vertical axes were set as [*hh*0] and [00*l*], respectively, where *h* and *l* are Miller indices. In Fig. 3(a), two reflections from Si and SiGe can be clearly identified. It is seen that the SiGe {224} reflection is highly asymmetric and elongated, showing that the SiGe layer contains mosaic structures. This is believed to be introduced during relaxation process due to the introduction of misfit dislocations. Reflecting the asymmetric feature of the SiGe {224} reflection, the Si {224} reflection is also asymmetric. Since the Si {224} reflection contains contributions from the Si substrate and Si thin film, the mosaic structures appeared in the SiGe virtual substrate is considered to be transferred in the epitaxial Si layer, leading to the elongation of the Si {224} reflection. On the other hand, three peaks can be seen in Fig. 3(b), which come from the SiGe buffer

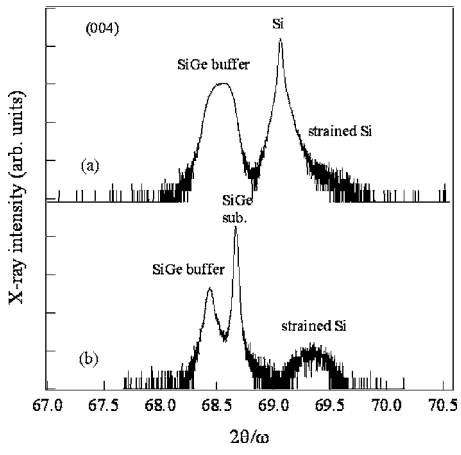

FIG. 2. Comparison of x-ray diffraction of {004} $2\theta/\omega$ scans of strained Si (a) on the SiGe virtual substrate and (b) on the SiGe bulk substrate.

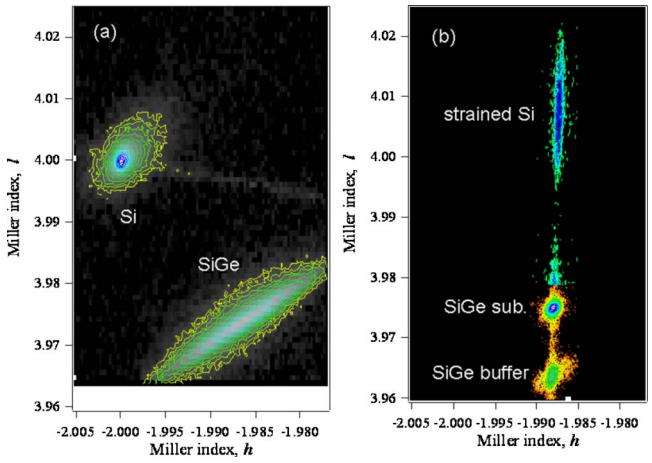

FIG. 3. (Color online) Comparison of x-ray reciprocal space mapping around {224} of strained Si for (a) on the SiGe virtual substrate and (b) on the SiGe bulk substrate.

layer, the SiGe substrate, and the strained Si thin film from the smaller Miller index, *l*, respectively. Importantly, these three reflections are vertically aligned, showing that both the SiGe buffer layer and the Si layer are pseudomorphically grown on the SiGe bulk substrate, and the epitaxially grown film is fully strained. No broadening to the lateral direction is observed in the Si {224} reflection. This is in contrast to that of the virtual substrate, and shows that the mosaicity in the strained Si layer on the SiGe bulk substrate was drastically reduced compared with that on the SiGe virtual substrate.

To have access to the strain fluctuation in the microscopic scale, microscopic Raman spectroscopy was performed. Raman spectra were measured at 100 points of each sample, and the peak positions of the Si–Si mode in strained Si and SiGe were extracted from each spectrum. Figure 4 shows the relationship between the two Si–Si modes in (a) the sample on the SiGe virtual substrate and (b) that on the SiGe bulk substrate. It is obvious that the fluctuation of the strain in the Si thin film is dramatically suppressed by utilizing the SiGe bulk substrate. In fact, the standard deviation in the peak position of the strained Si layer was decreased from 0.48 to 0.25 cm^{-1} by utilizing the SiGe bulk substrate. Therefore, it is concluded that the SiGe bulk substrate can be utilized as a substrate for strain-controlled heterostructures, which would be promising to investigate the inherent properties without suffering from the structural imperfection.

However, it should be pointed out that further improvement in the bulk crystal quality must be realized to routinely obtain SiGe bulk substrates. In fact, a part of the substrates obtained from the SiGe bulk crystal was found to contain slightly misoriented domains as evidenced by the peak splitting in the x-ray reciprocal space mapping (data not shown). Due to the lattice mismatch between Si and Ge, the variation of the alloy composition in the bulk crystal results in the introduction of strains. To release the built in strain, polycrystallization is sometimes observed. In addition, the constitutional supercooling in the SiGe melt as well as the inhomogeneous nucleation at the crucible wall could lead to the polycrystallization. Further study is necessary to fully establish a crystal growth technology to obtain high-quality SiGe bulk crystal with uniform composition.

In summary, we attempted to utilize homemade SiGe bulk crystal as a substrate for subsequent epitaxy of strained

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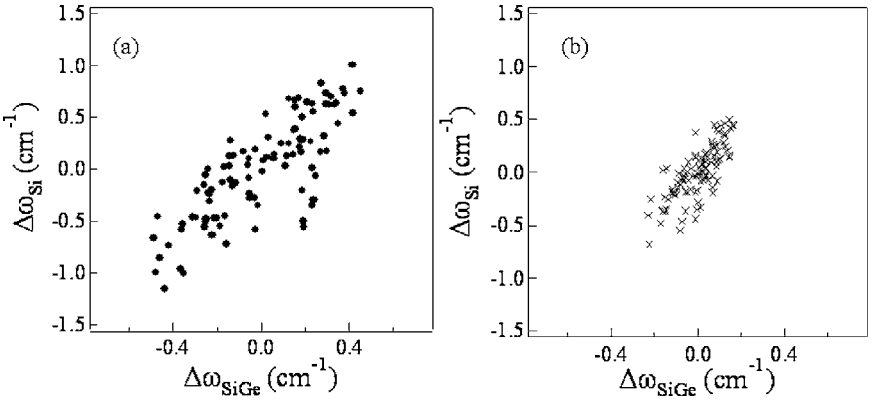

FIG. 4. Relationship between the Si–Si modes in strained Si and SiGe for (a) the sample on the SiGe virtual substrate and (b) that on the SiGe substrate.

Si thin film. X-ray reciprocal space mapping of asymmetric {224} diffraction clarified that the growth of a Si thin film on the SiGe bulk substrate leads to reduction in the orientation fluctuation compared with that on the SiGe virtual substrate. Furthermore, analysis of Raman spectra revealed a dramatic decrease of the strain fluctuation in the strained Si film by utilizing the SiGe bulk substrate. These results suggest that the SiGe bulk crystal can be utilized as a substrate for various strain-controlled group-IV heterostructures for fundamental studies as well as improvement of device performance.

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