# Ultrahigh Electron Mobilities in $Si_{1-x}Ge_x/Si/Si_{1-x}Ge_x$ Heterostructures with Abrupt Interfaces Formed by Solid-Phase Epitaxy

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## 1. Introduction

The application of Si<sub>1-x</sub>Ge<sub>x</sub> / Si / Si<sub>1-x</sub>Ge<sub>x</sub> heterostructures in Si devices is highly advantageous because of their higher potential carrier mobilities [1-4] compared to those in conventional Si devices. However, the electron mobilities reported to date have not come close to the ideal value [5]. To realize ultrahigh electron mobilities, it is essential to form an abrupt interface at the top of the channel where the electron confinement occurs, while also reducing the defect density within the channel. Consequently, precise control of the intermixing between Si and Ge at the interface is important, but this cannot be realized through conventional molecularbeam epitaxy (MBE) techniques.

We have developed a new growth method that combines MBE and solid-phase epitaxy (SPE). With this method, we have fabricated what appears to be an atomically flat interface between the channel and the doped region, and due to this interface we could obtain ultrahigh mobility of  $5.5 \times 10^5$  cm<sup>2</sup>V<sup>1</sup>s<sup>-1</sup> at 4.2 K.

### 2. Experimental Procedure

A schematic cross-section of the heterostructure used in the experiment is shown in Fig. 1. The p-Si (100) substrates were cleaned by chemical etching followed by thermal cleaning in a UHV chamber. A thick Si<sub>1-x</sub>Ge<sub>x</sub> (0.1 $\leq x\leq 0.4$ ) buffer layer (0.5-2 µm thick) was then grown at 600°C to minimize the strain caused by the lattice mismatch between the buffer layer and the substrate. Two types of buffer layer were used: (1) a single layer with a constant Ge content (x), or (2) a stacked layer combining the constant Ge content (x) layer with a graded Ge content ( $0\leq y\leq x$ ) layer below it. Next, a Si channel layer (20 nm thick) was grown at 400°C. This layer was as thick as possible, within the critical value for pseudomorphic growth of Si on Si<sub>1-x</sub>Ge<sub>x</sub> (0.2 $\leq x\leq 0.3$ ), to eliminate the surface roughness of the buffer layer.

Above the channel layer, a Si<sub>1-x</sub>Ge<sub>x</sub> spacer layer, an Sb delta-doping layer and a Si<sub>1-x</sub>Ge<sub>x</sub> cap layer were formed by SPE to avoid any surface segregation of Ge and Sb; i.e., each layer was deposited below 100°C then crystallized at 600°C. Last, a Si cap layer was grown at 600°C.

The strain field and microstructures in the heterostructures were characterized by Raman spectroscopy and cross-sectional transmission electron microscopy. The transport properties of the channel were evaluated by Hall-effect measurement at 4.2 K.

### 3. Results and Discussion

The Raman shifts related to Si-Si vibration in the

heterostructures are summarized in Fig. 2 as a function of the buffer-layer thickness and Ge content (x). The strain in the channel was evaluated from the Raman shift assuming Begard's law. The conduction band discontinuity was calculated from the strain in the channel using the procedure proposed by People *et al.* [6] and van de Walle *et al.* [7]. These values are indicated on the right axes in Fig. 2.

In the samples with the 0.5-µm-thick buffer layers, the strain was lower than in the other samples with thicker buffer layers (1.0 or 2.0 µm thick). This suggests that the strain relaxation was insufficient in the 0.5-µm-thick buffer layers. In the other samples, the strain relaxation seems to have been almost complete because there is little difference in the Raman shifts for the samples with different buffer-layer thicknesses.

The cross-sectional transmission electron microscopic image for a typical sample with the graded buffer layer  $(x=0.2, 0 \le y \le x)$  is shown in Fig. 3. Misfit dislocations were limited to the bottom part of the buffer layer and the substrate. No threading dislocations were observed in or around the channel layer. The high-resolution image indicated that the heterointerfaces were very smooth and flat. These features are similar to those observed in the sample without the graded buffer layer.

The electron mobilities  $(\mu)$  for the samples with or without the graded buffer layer are summarized in Fig. 4 as a function of Ge content (x) and the carrier concentration (n) which is controlled by the Sb doping level. All the mobilities increased proportionally with increasing *n* suggesting the nature of a two-dimensional electron gas. In addition, the mobility for the sample with the graded buffer layer was nearly one order of magnitude higher than the mobility without the graded buffer layer. Ultrahigh mobility of  $5.5 \times 10^5$  cm<sup>2</sup>V<sup>-1</sup>s<sup>-1</sup> was obtained at  $n=1.6 \times 10^9$  cm<sup>-2</sup> for the sample with the graded buffer layer (*x*=0.2), which is the highest value for SiGe / Si heterostructures reported to date.

We do not understand yet why the mobilities of the samples with the graded buffer layer were always higher than those without the graded buffer layer even though the electron microscopic observation showed no differences between the two types of sample. We are now planning a detailed examination of atomic-scale roughness at the channel surface. Also, note that the mobilities for all of our samples, even without the graded buffer layer, were higher than those previously reported for similar structures [1, 2]. This suggested that the interface mixing between Si and Ge was drastically suppressed by the SPE process we used. This method combining MBE and SPE promises to be a powerful tool for realizing sophisticated high-speed SiGe devices.

### 4. Conclusion

We successfully fabricated  $Si_{1,x}Ge_x / Si / Si_{1,x}Ge_x$ heterostructures with a flat channel. Thick graded buffer layers grown by MBE enabled us to control the strain field and realize large conduction band discontinuities. In addition, the SPE growth completely suppressed Ge segregation between the channel layer and the doped layer. As a result, ultrahigh electron mobility  $(5.5 \times 10^5 \text{ cm}^2 \text{V}^{-1} \text{s}^{-1} \text{ at } 4.2 \text{ K})$  in the  $Si_{1,x}Ge_x / Si / Si_{1,x}Ge_x$  heterostructure was obtained.

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| Si cap (5 nm)  |
|--|
| Si <sub>1-x</sub> Ge <sub>x</sub> (15 nm)<br>Si <sub>1-x</sub> Ge <sub>x</sub> (15 nm) |
| Si channel (20 nm)   |
| Si <sub>1-x</sub> Ge <sub>x</sub> buffer (0.5, 1.0 μm) uniform composition             |
| Si <sub>1-y</sub> Ge <sub>y</sub> buffer (0.0, 1.0 µm) compositionally graded          |
| Si buffer (50 nm)  |
| p-Si (100) substrate   |

Fig. 1 Cross-section of the SiGe / Si / SiGe heterostructure



Fig. 3 Cross-sectional transmission electron microscopic images of a heterostructure with a graded buffer layer (x=0.2, 0≤y≤x). A high-resolution image from the channel region is shown at the top of the figure.

#### References

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Fig. 2 Raman shifts related to Si-Si vibrations and strain as a function of Ge content for heterostructures with various types of buffer layers; ○: uniform 0.5-µm-thick buffer layer, □: uniform 1.0-µm-thick buffer layer, ■: combination of 1.0µm-thick uniform buffer layer and 1.0-µm-thick compositionally graded buffer layer



Fig. 4 Electron mobilities as a function of carrier concentration for heterostructures with various types of buffer layers.