Abrupt Si/Ge/Si(001) Interfaces Fabricated with Bi as a Surfactant

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While the effectiveness of surfactants in Si/Ge heteroepitaxy has recently been demonstrated, their disadvantages of self-incorporation and poor surface morphology restrict their practical application. We propose Bi as a surfactant that overcomes these disadvantages. We present that abrupt Si/Ge/Si(001) interfaces are fabricated using Bi while the amount of Bi incorporated is smaller than the detection limit of SIMS instrument ($<5x10^{16}$ cm⁻³).

1. Introduction

Fabrication of future electron devices based on Si/Ge heterostructure is an attracting challenge to extend the limits of state-of-the-art Si technology. To realize an ideal interface in the Si/Ge system, intermixing of Ge and Si caused by three-dimensional (3D) islanding and surface segregation of Ge1-5) must be prevented. It has recently been shown that the surfactant epitaxy is promising approach.⁶⁻¹³) This technique, a however, has run up against heavy doping of the surfactant atoms in the epitaxial layers^{10,12}) which would restrict its practical application. It has also shown that the surface diffusion of the growing species is suppressed in the presence of a surfactant which prevents the Ge 3D islanding but increases the surface step density during Si growth.¹⁴⁻¹⁶⁾ This means that a surfactant improves abruptness but degrades flatness of Si/Ge/Si interfaces. From the former point of view, incorporation of an applicable surfactant in Si or Ge should be as small as possible. If incorporated, it should not be harmful to electrical properties. From the latter point of view, a surfactant should be used only in case of need, and it should be easily removable. We selected Bi based on the above criteria. Bi has one of the smallest segregation coefficient and the smallest solid solubility among the group III and V elements for melt growth of Ge and Si. Bi atoms occupy the Si(001) surface up to a saturation coverage at 400 °C and desorb completely above 580 °C. In this presentation, we use Bi as a

surfactant and show that abrupt Si/Ge/Si(001) interfaces can be fabricated with very low Bi doping in the epitaxial layers.

2. Experiment

We used an ion-pumped Si MBE system with an electron-beam evaporator for Si and resistively heated effusion cells for Ge, Sb and Bi. A well-oriented Si(001) substrate was subjected to a standard cleaning process¹⁷) and was loaded into the growth chamber. After removal of the protective oxide film, an atomically clean starting surface was produced by deposition of a Si buffer layer at 700 °C and a subsequent 1000 °C anneal. A 30 keV RHEED system was used for surface analysis. The electron microscopy was carried out using a 200 kV electron microscope. SIMS measurements were made with O₂+ primary ions of 3 keV, 80 nA for detecting ⁷⁴Ge, ¹²³Sb and ²⁰⁹Bi secondary ions.

3. Results and discussion

Figure 1 shows RHEED intensity evolution of the specular beam during growth of a Ge/Bi/Si(001) structure. The Bi coverage was nearly 1 ML. In the growth without Bi (upper trace), the intensity oscillation damps rapidly after the fifth peak, which represents the change in growth from layer-by-layer to 3D islanding as shown by RHEED patterns inset.¹⁸) With Bi as a surfactant (lower trace), on the other hand, the intensity oscillation lasts more than 12 periods and





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Fig. 2. Cross sectional TEM images of Si/10ML Ge/Si(001) buried structure grown at 400 °C without surfactant (a) and with a Bi adlayer (b).

no trace of 3D islanding is seen in the RHEED pattern. This indicates that the Ge layer grows in a layer-by-layer mode up to 12 ML instead of the 3D islanding.¹⁵)

Figure 2 shows cross sectional TEM images of Si/10ML Ge /Si(001) structure. Ge atoms were aggregated to form islands without Bi (a), while a Ge layer with uniform thickness was fabricated with a Bi adlayer.

Figure 3 shows SIMS profiles of samples consist of four Ge layers of 4 ML thick separated by 30 nm Si layers. Sb (a) or Bi (b) atoms for a saturation coverage (~1 ML) were deposited once on the surface of the third Ge layer. In both samples, leading edges of the Ge layers grown after the surfactant adsorption become steeper, indicating that the Sb and Bi adlayer improve the abruptness of Si/Ge interface by suppressing the Ge surface segregation. It should be noted that the Sb concentration in the epitaxial layer is as high as $2x10^{19}$ cm⁻³, while the amount of Bi incorporated is smaller than the detection limit of the SIMS instrument (< $5x10^{16}$ cm⁻³).

Figures 4a and 4b show cross sectional TEM images of the fourth and second Ge layers of the sample of Fig. 3b, respectively. In Fig. 4b, the Si/Ge interface grown without Bi is smeared out by the surface segregation of Ge atoms. The Ge/Si interface is, on the contrary, observed to be smooth and flat. For the fourth layer grown with Bi (Fig. 4a), the Si/Ge interface is distinct and the width of dark band becomes narrower indicating improvement of interface abruptness. the However, indented atomic steps are clearly observed at both Si/Ge and Ge/Si interfaces suggesting that surface smoothness was degraded during the Si growth due to the surfactant effect.



Fig. 3 . SIMS profiles of Si/Ge/Si(001) heterostructure. Sb (a) or Bi (b) atoms (~1 ML) were adsorbed on surface of the third Ge layer (shown by an arrow) during the growth at 400 °C.

4. Conclusion

We have demonstrated that Bi layer adsorbed on the surface preserves layer-by-layer Ge growth up to 12 ML and reduces the intermixing of Si and Ge caused by surface segregation. It was found that a major effect of a surfactant is to reduce the surface mobility of the growing species which consequently restrict islanding at the sacrifice of surface morphology. Among the elements that is an effective surfactant for the growth of Si/Ge system, Bi is an excellent one realizing small self-incorporation and controllable adsorption and desorption on Si(001).



Fig. 4. Cross sectional TEM image of 4ML Ge layers embedded in Si: (a) grown with Bi as a surfactant (the fourth Ge layer in Fig.3b), (b) grown without Bi (the second layer in Fig.3b).

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