Erbium and Germanium Profiles in Si_{1-x}Ge_x Layers Grown by Silicon Sublimation-Source Molecular-Beam Epitaxy in GeH₄

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Abstract—The Ge and Er depth profiles in $Si_{1-x}Ge_x$ layers grown on Si(100) substrates by Si sublimationsource molecular-beam epitaxy in GeH₄ were studied by secondary ion mass spectrometry. The results demonstrate that Ge facilitates Er incorporation into the growing Si–Ge layer. The Er dopant profile becomes sharper with increasing Ge content. The Ge profile also has rather sharp boundaries, indicating that there is no Ge surface segregation, which is attributable to the presence of adsorbed hydrogen, acting as a surfactant.

INTRODUCTION

Rare-earth doped silicon is of considerable technological interest because it exhibits efficient luminescence at 1.54 μ m, the wavelength corresponding to the lowest dispersion in silica fibers. Ennen *et al.* [1] and Stimmer *et al.* [2] reported room-temperature electroluminescence from diodes based on silicon structures which were doped with erbium during molecular-beam epitaxy (MBE). In recent years, attention has also been paid to the study of Er-doped silicon–germanium layers [3], which are potentially attractive for developing Sibased lasers.

However, Er doping of Si–Ge layers has been studied less deeply compared to Si layers. Little or no data on the dopant distribution in Er-doped MBE Si–Ge layers are available in the literature. The Er dopant in Si layers was reported to be subject to surface segregation [4, 5]. Similar behavior might be expected in Er-doped Si–Ge layers.

In producing Er-doped Si layers, oxygen incorporation activates the Er trapping by the growing layer [4]. At the same time, since the Ge flux is difficult to stabilize in the MBE process, it is more attractive to grow Si–Ge layers with the use of gas sources [6], without admitting oxygen to the deposition chamber.

The objective of this work was to study the Er trapping by the growing Si–Ge layer and to examine the possibility of producing steep doping profiles by sublimation-source MBE in GeH_4 .

EXPERIMENTAL

Heterostructures were grown by Si sublimationsource MBE in GeH_4 as described previously [7]. The atomic Si flow was produced via sublimation of an Si single crystal. GeH_4 decomposed on the growth surface, ensuring Ge incorporation into the growing layer. The Er source used was single-crystal Er-doped Si. The layers were deposited on Si(100) substrates.

The structures included an ~100-nm-thick buffer layer grown at a substrate temperature of 1000°C, followed by an Si–Ge layer of equivalent thickness 50 to 100 nm deposited at 500°C and capped with undoped silicon.

The Ge, Er, and O depth profiles in the grown layers were measured by secondary ion mass spectrometry. The Ge content of the layers was determined by x-ray diffraction (XRD).

RESULTS AND DISCUSSION

Figure 1 shows the Ge, Er, and O depth profiles in Si/Si_{1-x}Ge_x(Er)/Si(100) heterostructures. The first heterostructure was grown at $p_{\text{GeH}_4} = 2.7 \times 10^{-3}$ Pa using an Er-doped Si source, with no cap layer. It can be seen in Fig. 1a that the Ge concentration rises steeply starting from the buffer layer. In the transition region, the Ge concentration increases by about one order of magnitude every 14 nm. The Ge concentration is nearly constant at 3×10^{21} cm⁻³ (x = 0.06) in the interior of the



Fig. 1. Ge, Er, and O depth profiles in $Si/Si_{1-x}Ge_x\langle Er \rangle/Si(100)$ heterostructures grown using an Er-doped Si source at $p_{GeH_4} = (a) 2.7 \times 10^{-3}$ (no cap layer) and (b, c) 10.6×10^{-4} Pa; (c) the substrate is biased by -300 V.

layer and is slightly lower in the surface region. A similar Ge content (x = 0.07) was inferred from XRD data. The Er and Ge profiles are similar in shape. The Er concentration in the layer approaches that in the source ($\sim 5 \times 10^{18}$ cm⁻³). Note that, in Si layers grown from similar sources without admitting oxygen to the deposition chamber, the Er concentration is no higher than $\sim 10^{17}$ cm⁻³ [8].

At a lower germane pressure, $p_{\text{GeH}_4} = 10.6 \times 10^{-4}$ Pa, the Ge content of the Si_{1-x}Ge_x layer is much lower, $x \sim 0.01$ (Fig. 1b). The Ge concentration varies

strongly across the Si_{1-x}Ge_x layer: near the cap layer, it is about half as high as at the interface with the buffer layer. In the cap layer, grown without admitting GeH₄ to the chamber, the Ge concentration is still lower. The depth profile of Er in the Si_{1-x}Ge_x layer is similar in shape to that of Ge. The Er concentration rises by about one order of magnitude every 25 nm near the buffer layer and drops more steeply, by about one order of magnitude every 9 nm, toward the cap layer.

A voltage of -300 V applied to the substrate during $Si_{1-x}Ge_x\langle Er \rangle$ MBE notably raises the Ge content (x = 0.09) (Fig. 1c). The Ge concentration rises by about one order of magnitude every 12 nm near the buffer layer and decreases by about one order of magnitude every 8 nm as the cap layer is approached. The Er profile across the $Si_{1-x}Ge_x$ layer has a similar shape. The Er concentration is comparable to that in the other heterostructures.

A few features of our experimental data warrant attention. The highest Er concentration in the grown layers is $(3-4) \times 10^{18}$ cm⁻³, independent of the Ge content of Si_{1-x}Ge_x. The Ge concentration in the Si_{1-x}Ge_x layer varies more steeply at higher p_{GeH_4} and also when a negative bias is applied to the substrate. The Ge concentration changes by about one order of magnitude every 8–9 nm near the Si/Si_{1-x}Ge_x interface and every 12 nm near the buffer layer/Si_{1-x}Ge_x interface, indicating that we obtained Ge profiles with rather sharp boundaries. The sharpness of the Ge profile at the Si/Si_{1-x}Ge_x⟨Er⟩ interface is limited by the fact that p_{GeH_4} decreases only gradually after the GeH₄ supply is cut off, and Ge incorporation into the growing layer continues until all of the residual GeH₄ is pumped out.

Ge trapping by the growing Si layer proceeds in the same way as in the case of other dopants in the MBE process [9]. Initially, a Ge adlayer forms on the surface of the growing layer, ensuring Ge incorporation into the layer. Owing to the surface segregation of Ge, the boundary of the Si_{1-x}Ge_x layer is rather broad.

The present results demonstrate that, in the process of Si sublimation in GeH₄ at a growth temperature of ~500°C, Ge segregation is insignificant. This is probably due to the formation of a continuous surface layer of hydrogen resulting from GeH₄ dissociation. Surface hydrogen may influence the kinetics of Ge segregation during the growth of Si/Si_{1-x}Ge_x heterostructures, suppressing surface segregation. The adsorbed hydrogen acts as a surfactant [6].

Since the Si flow from the sublimation source contains Si⁺ ions, a negative bias applied to the substrate accelerates the transport of these ions to the substrate surface. The Si⁺ ions interact with Ge, Er, and O atoms, facilitating their incorporation into the growing layer [8]. The fact that the Er profile becomes sharper with increasing Ge content indicates that Ge influences the surface segregation of the Er dopant.

CONCLUSION

The present results demonstrate that, in the sublimation-source MBE of Si_{1-x}Ge_x(Er)/Si(100) heterostructures in GeH₄, Ge facilitates Er incorporation into the growing Si–Ge layer. The Er concentration profile becomes sharper with increasing Ge content. The Ge profile also has rather sharp boundaries, indicating that there is no Ge surface segregation. This is probably due to the presence of hydrogen, which results from GeH₄ dissociation and passivates the growth surface.

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