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Improvement of crystallinity by post-annealing and regrowth of Ge layers on Si substrates

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ABSTRACT

Post-annealing and regrowth of Ge were investigated to improve the crystallinity and to control the lattice strain of Ge layers directly grown on a Si substrate by low-temperature epitaxial growth. The post-annealing at a higher temperature was an effective way of improving the surface morphology and the crystallinity of the Ge layers. Furthermore, the lattice strain changed from compressive to tensile in <110> crystal orientation when the post-annealing temperature was increased, and the tensile strain of 0.19% was achieved at the annealing temperature of 700 °C. Consequently, the photoluminescence (PL) intensity increased with the increasing post-annealing temperature and a red-shift of the PL spectra could be observed due to reduction of direct bandgap energy at Γ-point with the tensile strain. Although regrowth of the Ge layers had little impact on the lattice strain at a relatively low regrowth temperature, a thick Ge layer with high crystallinity was formed at 700 °C and a favorable PL spectrum was obtained. These results indicate that this combined technique can improve the performance of Ge light-emitting devices.

1. Introduction

Silicon photonics are attracting attention as a key technology for chip-to-chip or on-chip optical interconnections to overcome the density of transmitted data and power consumption in metal lines in large-scale integrated circuits [1,2]. Optical devices such as light emitters [3–6], optical receivers [7,8], waveguides [9], modulators [10,11], and photo-multiplexers/de-multiplexers [12] can be stably fabricated by fine Si processes.

Since Si and Ge, which are commonly used in standard Si processing, are indirect bandgap materials, the fabrication of the on-chip light source has been a great challenge. Various methods have been attempted for integrated light sources that can be fabricated with complementally metal-oxide-semiconductor logic circuits by using the quantum size effect [13], heterostructures [14], and other processes [15–17]. One of the most promising devices of these approaches involves germanium lasers for improving the quantum efficiencies with highly n-type doping and tensile strain in the Ge active regions [18,19]. However, since the lattice constant of Ge is 4.2% larger than that of Si, if a Ge layer is grown on a Si substrate, crystal defects such as dislocation are generated at the Ge/Si interface due to the strain relaxation. The Ge epitaxial growth on Si substrate without any thick buffer layers has recently been achieved for metal-oxide-semiconductor field effect transistors [20,21] and for photodetectors [7,8], and improved crystallinity in Ge layers has been studied using cyclic annealing [22], high temperature annealing [23], and low temperature buffer layers [24]. However, the threading dislocations and non-radiative recombination centers must be further decreased to improve luminous efficiency. Furthermore, although highly n-type doping has been recognized as an effective way of improving the direct transitions at the Γ-point, due to filling the conduction band minimum with electrons at the L-point [18,19], the crystallinity of the Ge layers degrades when doping concentration is high. Thus, the doping concentration is limited to about the order of 10^{19} cm^{-3} with acceptable crystallinity and surface morphology [25]. Another attempt involves improving the quantum efficiency with the tensile strain to the Ge layer [26], and although it has been reported that the Ge layers contain a tensile strain after high temperature annealing due to the difference of thermal expansion coefficients [26–28], systematic studies have not yet been carried out.

In this study, we investigated the effects of a combination of Ge epitaxial growth and post-annealing on the crystallinity and the lattice strain in order to improve the optical properties of the Ge layers.

2. Experimental details

The Ge was epitaxially grown by using a cold-wall rapid thermal chemical vapor deposition system. Germane (GeH_4) was used as a source gas, which was supplied with H_2 carrier gas. An eight-inch Si

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(100) CZ wafer was used as the substrate, which was initially treated by RCA cleaning, HF wet etching of the SiO_2 layer, and hydrogen termination of the wafer surface by rinsing in de-ionized water. Then, the wafer was annealed in a hydrogen atmosphere at 850 °C for 2 min. as a pre-cleaning process just before the Ge growth. It was confirmed that there were no contaminants such as oxygen and carbon on the wafer surface after the pre-cleaning process. As the starting point of improving the crystallinity and controlling the lattice strain, Ge layers with good surface morphology were grown at 420 °C under relatively higher pressure of 7000 Pa. Then, the Ge layers were annealed in the same H_2 atmosphere to improve the crystallinity. Although heat-up rate for the annealing was controlled in about 5 °C/s, the wafer was simply cooled in H_2 flow after the annealing, so the maximum cool-down rate of −20 °C/s was obtained just after the end of the annealing.

Surface morphology of the annealed Ge layers was evaluated by an atomic force microscope (AFM) [Veeco, Multimode in tapping mode with 1–10 Ω cm P-doped Si cantilever]. Crystallinity and lattice strain of the Ge layers were evaluated by high-resolution X-ray diffraction (XRD) analysis [Panalytical, X'Pert Pro with Bragg-Brentano geometry] and micro-Raman spectroscopy [Tokyo Instruments, Nanofinder]. We use a Cu $K\alpha_1$ X-ray source for the XRD measurements. Moreover, the crystallinity and optical properties of the Ge layers were also investigated by micro-photoluminescence (PL) spectroscopy [Tokyo Instruments, Nanofinder]. Raman and PL spectroscopies were carried out with an Ar laser in which the pumping wavelength was 457.9 nm.

3. Results and discussions

Fig. 1 shows a reciprocal space map (RSM) of XRD (XRD-RSM) from the 130-nm-thick Ge layer directly grown on the Si substrate. An AFM image of the Ge layer is also shown in the inset. A relatively good surface morphology of the Ge layer was achieved: the root mean square (RMS) roughness was 1.02 nm for the measured area of 2 μm × 2 μm. In the XRD-RSM, an intense Si (-1-13) peak was observed, which represented the diffraction from the Si substrate under the Ge layer. Since the XRD-RSM was measured by using semiconductor array detectors, errors in the counts occur if the diffraction intensity is very high; therefore, the streak line observed around the Si (-1-13) peak does not represent any actual diffraction. Although the thicknesses of the Ge layer was only 130 nm, a diffraction peak from Ge (-1-13) could be clearly observed, which means that the single crystalline Ge layer was obtained by using low-temperature epitaxial growth. Furthermore, since the position of the diffraction peak from the Ge layer was close to that from the unstrained Ge, it was confirmed that the lattice strain in the Ge layer originated from the lattice mismatch between Si and Ge was almost completely relaxed. However, the displacement of the diffraction peak shows that the as-grown Ge layer still contained a compressive strain just after the low temperature epitaxial growth at 420 °C due to the larger lattice constant of Ge compared to that of the Si substrate.

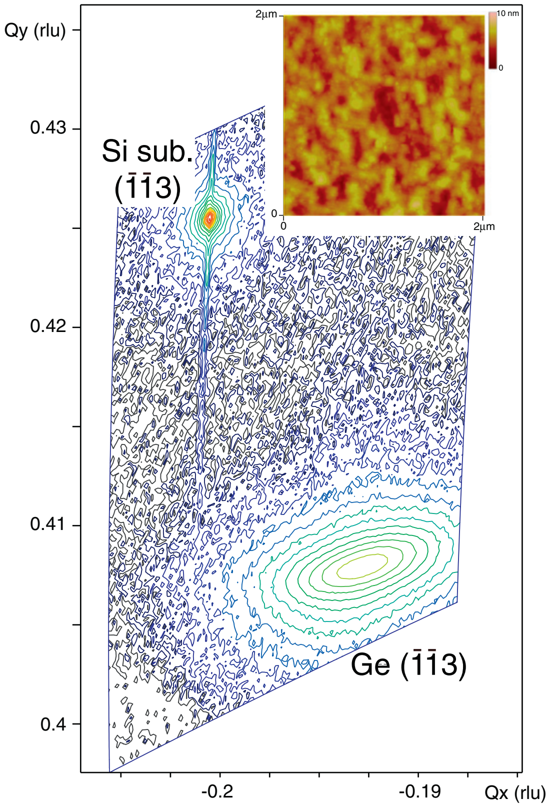

Fig. 1. XRD-RSM of (-1-13) diffraction from as-grown Ge layer on Si substrate. The inset shows AFM image of Ge layer grown on Si substrate.

3.1. Effect of post-annealing

Several approaches have been investigated to improve the crystallinity of Ge layers grown on the Si substrates [22–24], and it has been reported that cyclic annealing at a relatively higher temperature can reduce the threading dislocation density [22] in the Ge layers. This has led to studies on the effect of annealing on the crystallinity and the lattice strain of Ge layers. After the low temperature epitaxial growth of the Ge layers at 420 °C, the temperature was increased to the annealing temperature in the same H_2 atmosphere as that during the epitaxial growth, and the Ge layers were then annealed at certain temperatures for 10 min.

XRD-RSM and AFM images of the Ge layers annealed at various temperatures (T_a) after the low temperature epitaxial growth are shown in Fig. 2. Although the surface morphology of the Ge layer annealed at 500 °C (Fig. 2a) was almost the same as the as-grown Ge layer (Fig. 1), the short-range roughness had vanished and long-range undulations appeared after annealing at 600 °C (Fig. 2b). Moreover, some dimples were observed on the surface in addition to the long-range undulations after annealing at 700 °C (Fig. 2c). Despite having almost the same RMS value of the surface roughness, it was obvious that the short-range roughness could transform into the long-range undulations by the post-annealing at temperatures above 600 °C, which increased the area ratio of the relatively flat surface.

As shown in the XRD-RSMs, the Ge (-1-13) diffraction peaks became steeper and the peak intensity increased when the annealing temperature was increased, indicating that the crystallinity of the Ge layers was increased by the post-annealing. Fig. 3 shows the lattice strain in the Ge layers in the <001> and <110> crystal orientations as a function of the annealing temperature. Since the growth time for the low temperature epitaxial growth was long enough relative to the time of post-annealing, the lattice strain of the Ge layer annealed at $T_a = 420$ °C was the same as that of the as-grown Ge layer. The lattice strain in the <110> crystal orientation increased as T_a increased, and the strain in the <001> crystal orientation showed an opposite dependence. Although the Ge layer contained the compressive strain in the <110> crystal orientation at $T_a = 420$ °C, this strain started decreasing when T_a was increased, and the Ge was completely un-strained at $T_a = 530$ °C. Furthermore, the direction of the lattice strain changed from compressive to tensile after annealing at $T_a > 530$ °C, and the tensile strain at $T_a = 700$ °C reached 0.19%. This result is consistent with previous studies [29]. Normally, a grown layer with a larger lattice constant compared to a substrate contains a compressive strain within the growth plane. However, since the Ge layers grown on the Si substrate were almost completely relaxed even after low temperature growth, the Ge lattice could be dislocated at the Ge/Si interface by post-annealing, and the lattice strain of the Ge layer was relaxed during annealing at the relatively higher temperature with the volume determined by the thermal