Growth of high quality Ge-on-Silayer by using an ultra-thin LT-Si buffer in RPCVD

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Abstract. Ge epitaxial layer on Si substrate becomes more attractive for Si-based monolithic photonic integrated circuit (PIC). Low threading dislocation density and low surface roughness play a vital role in realizing the fabrication of the Ge optoelectronic devices. In this study, an ultra-thin LT-Si buffer for the deposition of Ge layer was investigated with regard to Ge layer’s crystallinity, symmetrical characteristic, threading dislocation density, and surface roughness. As a result, Ge epitaxial film has low threading dislocation density (TDD=5×10^6 cm^-2) and smooth surface (RMS=0.68nm) in 5µm×5µm scan field with the Ge epitaxial layer thickness of about 1µm. What’s more, it was grown in a short time by using an ultra-thin LT-Si buffer layer without using chemical mechanical polishing (CMP), high temperature annealing, H2 annealing or cyclic annealing. In addition, room temperature direct gap photoluminescence was observed from intrinsic tensile-strained (0.21%) Ge-on-Si layer and bandgap narrowing in Ge epitaxial layer is 85meV.

1. Introduction
Epitaxial growth of Ge layer on Si has brought great interest for Si-based monolithic optoelectronic integration [1-2] and novel CMOS device applications [3]. Ge layers on Si can also be utilized to the formation of Ge-on-insulator (GeOI) [4] based metal oxide semiconductor field effect transistors (MOSFETs) with high hole mobilities. In addition, Ge layers can be employed as buffer layers for the fabrication of GaAs-based optoelectronic devices, such as laser diodes [5], solar cells [6], and high electron mobility transistors [7], etc. However, it is difficult to grow high tensile strained, low root-mean-square (RMS) and low threading dislocation density (TDD) Ge layers on Si due to the 4.2% lattice mismatch and the large thermal expansion coefficient between Ge and Si. In the early stage of single-crystalline Ge epitaxial layer on Si substrates, compositionally graded Si_{1-x}Ge_x alloys were used as buffer layers [8]. However, the compositionally graded Si_{1-x}Ge_x alloys technique are too thick (more than 10µm) to be coupled with Si optical waveguide. LT-HT (low temperature/ high temperature) technique is born at the right moment [9]. Nevertheless, the Ge layers grown by LT-HT technique possess high TDDs in the order of 10^8-10^9 cm^-2, which are harmful for the performance of optoelectronic devices. Consequently, high temperature annealing [10], H2 annealing [11], and cyclic thermal annealing [12] are used to reduce TDD. However, annealing process adds the extra thermal budget. Many ways were developed to modify the LT-HT technique, such as, introducing a thin SiGe buffer [13] and LT-HT ramp layer [14-15].
In this work, high quality Ge-on-Si layer with an ultra-thin LT-Si buffer was grown in RPCVD system. The Ge layer suffers tensile strain of 0.21%, TDD = 5×10^6 cm^-2 and RMS=0.68nm. In order to show crystal quality of the Ge layer, photoluminescence of direct band to band transition is measured. Room temperature direct gap photoluminescence was observed from intrinsic tensile-strained Ge-on-Si layer.

2. Experiments
Epitaxial growth of Ge on 6 in. p-type Si (100) wafers was carried out in a single wafer reduced pressure chemical vapor deposition (RPCVD) system. Si wafer was first cleaned used RCA solution, dried by pure N_2 and then wafer was transferred to the growth chamber. Before the deposition of epitaxial layer, the Si wafer was baked in H_2 at 1050°C for 2min to remove native oxide. Then, growth temperature was degraded to 400°C for the deposition of an ultra-thin LT-Si layer (10nm) using SiH_4. Afterwards, the Ge layer was grown and the precursor for Ge is 2% germane (GeH_4) diluted in H_2 balance. A three-step Ge deposition was introduced and the thickness of the epitaxial layer was 1µm. The three steps in the growth sequence were: (I) LT-Ge growth at 350°C to obtain a Ge seed layer and maintain a smooth surface layer; (II) LT to HT ramping from 350 to 650°C at a rate of 80°C/min and the flow of GeH_4 was reduced half to maintain a lower growth rate and distribute enough time induce the tensile strain in the Ge epitaxial layer; and (III) HT growth at 650°Cto achieve the intended thickness with a reasonable growth rate.

Scanning electron microscope (SEM) was used to determine the thickness of Ge epitaxial layer on Si. Atomic force microscope (AFM) was used for the determination of surface roughness. High Resolution X-Ray Diffraction (HR-XRD) patterns were recorded on a Phillips X’Pert diffractometer operating at 40mA and 40kV using Cu Kα1 radiation. ω-2θ scan was utilized to determine the crystallinity and strain analysis of the Ge layer and φ scan was also measured to determine the symmetrical characteristic of the Ge film.

3. Results and discussion
Cross section SEM image of Ge-on-Si layer is shown in Figure 1 (a) and the thickness of Ge epitaxial layer is 1µm. The surface roughness of 1um thick Ge without annealing measured by AFM is shown in Figure 1 (b). RMS value of the Ge layer is 0.68nm. HR-XRD ω-2θ scan for Ge epitaxial layer grown on Si (100) without post-annealing at 20°to 90°scanning range is shown in Figure 2 (a). It shows a strong Ge (004) peak indicating no Ge diffraction peak of other orientations. HR-XRD ω-2θ scan around Si (004) and Ge (004) diffraction (at 64° to 71° scanning range) of 1µm thick Ge layer was also presented in Figure 2 (b). The Ge (004) peak position is 66.156° and the full width at half maximum (FWHM) of the Ge(004) peak is 0.06°. Comparing to the fully relaxed Ge (004) peak position of 20 = 66.004°, the peak shift is 0.152° and the Ge-on-Si layer is tensile strained by 0.283%, which is due to the difference of the thermal expansion coefficient of Si and Ge. During the process of growing LT-HT ramp layer, enough time was distributed to induce the tensile strain in the Ge epitaxial layer. The out-of-plane lattice constant parameter (a⊥) of Ge epitaxial layer from Ge (004) peak position (θ_{Ge}) can be extracted using Bragg’s law. It is expressed as:

\[
a^- = \frac{2\lambda}{\sin \theta_{Ge}}
\]  

(1)

The in-plane lattice constant (a//) of the Ge layer can be calculated by:

\[
a// = \frac{1+v}{2v} \left[ a_{Ge} - a^- \left( \frac{1-v}{1+v} \right) \right]
\]  

(2)
where $v$ is Possion’s ratio of Ge, $v=0.271$, and $a_{Ge}$ is the unstrained Ge lattice constant, $a_{Ge}=0.56578\text{nm}$. Therefore, the degree of strain relaxation $R$ can be reckoned as:

$$ R = \frac{a'' - a_{Ge}}{a_{Ge}} $$

Figure 3 shows the HR-XRD reciprocal space maps (RSM) of the range between Si and Ge (004), which demonstrates good crystallinity of the Ge epitaxial layer. In order to discuss the symmetrical characteristic of Ge crystal in epitaxial layer, HR-XRD $\phi$-scan around Si (022) and Ge (022) was carried out, as shown in Figure 4. The Si (022) scan shows the presence of peaks every 90°, as expected for the cubic Si symmetry. The Ge (022) shows the presence of peaks every 90°, indicating the four symmetry of Ge crystal, which verifies the good quality of Ge epitaxial layer.

**Figure 1** (a) Cross section SEM image of Ge-on-Si layer  
(b) AFM image of surface morphology of Ge layer deposited on Si (100) substrate

**Figure 2** HR-XRD $\omega$-20 scan for Ge epitaxial layer grown on Si (100) without post-annealing at (a) 20°to 90°scanning range and at 64°to 71°scanning range.
Figure 3 HR-XRD reciprocal space maps (RSM) around Si (004) and Ge (004) diffraction of 1um thick Ge-on-Si sample without annealing.

Micro-Raman spectra using 514nm Ar\(^+\) laser has been used to determine the crystal quality and the in-plane strained of the Ge epilayer. As shown in Figure 5, the Raman spectra ranging from 240-360cm\(^{-1}\) show that there is a red shift of Ge-Ge peak position compared to the bulk Ge, indicating that Ge layer is under tensile strain. The peak position is 300.27649cm\(^{-1}\) and the value of in-plane strained can be calculated by using the following expression:
\[ w(\text{cm}^{-1}) = 300.8 - 400\varepsilon, \]

The FWHM of the Ge-Ge mode peak is only 1.652 cm\(^{-1}\) comparing with bulk Ge 1.625cm\(^{-1}\).

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**Figure 5** Raman scattering spectra of bulk sample Ge and Ge-on-Si samples

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**Figure 6** Room temperature direct bandgap photoluminescence (PL) spectra of 1um thick Ge on Si without post-annealing.

Room temperature direct bandgap PL spectra from intrinsic tensile-strained Ge-on-Si layer was shown in Figure 6. Direct bandgap PL peak is located at 0.775eV (1600nm) and corresponding to the direct band-to-band optical transition from the direct T valley to the valence band. Comparing to the direct bandgap PL peak of bulk Ge (1520nm), the red-shift of direct bandgap PL peak was due to the tensile strain (0.28\%) of Ge-on-Si layer. Indirect band gap PL peak is observed at 0.69eV and the
bandgap narrowing in Ge epitaxial layer is 85meV, which illustrates the Ge layer may be applied to the Si-based monolithic photonic integrated circuit (PIC). In addition, we use the Secco defect etching to determine the TDD in the as-grown Ge layer, and I$_2$ solution (HF:HNO$_3$:CH$_3$COOH:I$_2$=5ml:10ml:11ml:30mg) was selected. The TDD = $5 \times 10^6$ cm$^{-2}$, was shown in Figure 7.

![TDD=5 × 10^6$cm^{-2}$](image)

**Figure 7** Optical image of the surface of the Ge layer after Secco etch

### 4. Conclusions
In conclusion, high quality Ge-on-Si layer has grown by using an ultra-thin LT-Si buffer in RPCVD system. We combined low LT-HT ramp rate method with LT-Si buffer technique, tensile strain (2.1%), low TDD ($5 \times 10^6$ cm$^{-2}$) and low RMS (0.68nm) Ge epitaxial layer was acquired without using high temperature annealing, H$_2$ annealing, cyclic thermal annealing and CMP. The growth sequences were: (I) LT-Si buffer; (II) LT-Ge seed layer; (III) LT-HT Ge ramp layer; (IV) HT-Ge layer. The crystallinity and symmetrical characteristic were verified by using HR-HRD $\omega$-2$\theta$ scan and $\varphi$-scan. FWHM of Ge diffraction peak was 0.06° and four symmetry of Ge crystal was observed, which indicating good quality of Ge epitaxial layer. In addition, room temperature direct bandgap PL spectra was measured. The bandgap narrowing in Ge epitaxial layer is 85meV, which illustrates the Ge layer may be applied to the Si-based monolithic photonic integrated circuit (PIC).

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