

# Hot-C<sup>+</sup>-Ion Implantation Optimization for Forming Nano-SiC Region at Surface (100)SOI Substrate

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## Abstract

We experimentally studied a hot-C<sup>+</sup>-ion implantation (HCI) optimization for forming nano-SiC regions in a (100)SOI substrate, to improve the photoluminescence (PL) emission for a future Si-based photonic device. We successfully optimized that the HCI temperature  $T$  is about 700°C and the C ion dose  $D_C$  is  $4 \times 10^{16} \text{ cm}^{-2}$  to realize strong PL intensity  $I_{PL}$  from an approximately 1.5-nm-thick C atom segregation layer (CSL) which is analyzed by an atom probe tomography (APT) at the surface oxide (SOX)/Si interface. Corrector-spherical aberration TEM (CSTEM) observation also showed that both a 4H- and 3C-SiC (silicon carbide) nano-areas are partially formed near both the SOX/Si and buried-oxide (BOX)/Si interfaces in the CSL, and PL photons are mainly emitted from these SiC areas.

## I. Introduction

Recently, we experimentally studied a Si<sub>1-y</sub>Cy layer fabricated by hot-<sup>12</sup>C<sup>+</sup>-ion implantation (HCI) into a (100)SOI at 900°C in a wide range of  $0.01 < Y \leq 0.25$  and  $0.5 \leq d_S \leq 20 \text{ nm}$ , where  $d_S$  is the SOI thickness [1], [2]. We demonstrated very large bandgap  $E_G$  ( $\approx 3 \text{ eV}$ ), and very strong  $I_{PL}$  from the near-UV to visible region ( $> 400 \text{ nm}$ ) of the Si<sub>1-y</sub>Cy layer, which drastically increases with increasing  $Y$  in  $Y \leq 0.25$ . C atoms segregate at both the SOX/Si and BOX/Si interfaces, resulting in partial formation of 3C-SiC at the BOX/Si interface [2]. Strong PL emission, which is about 100 times as large as that of 2D-Si [2], originate from the C segregation layer (CSL). Thus, the Si<sub>1-y</sub>Cy technique is very suitable for both a new  $E_G$  engineering for high-speed source-heterojunction devices (SHOT) [3] and visible Si-based photonic devices [4].

In this work, we experimentally optimized the HCI process of  $T$  and  $D_C$  of a Si<sub>1-y</sub>Cy layer at the surface (100) SOI substrate to realize stronger  $I_{PL}$  for a Si photonic device, as well as to study the nano-SiC quality in the CSL, using the analytical methods of ATP [5], CSTEM, and PL.

## II. Experiment Procedure

Si<sub>1-y</sub>Cy layers were fabricated by HCI into (100) bonded SOI substrate with an about 100-nm thick SOX [2], where  $2 \times 10^{16} \leq D_C \leq 7 \times 10^{16} \text{ cm}^{-2}$ . The peak recoil energy  $E_R$  of C<sup>+</sup> ions exists in the thick SOX, resulting in lower ion-implantation-induced-damage (IID) in the Si layer. In this work, we used the thin (8nm) and thick (20nm) Si layer of SOI substrate. The SOI substrate temperature  $T$  at HCI was varied from 500 to 1000°C, to study the nano-SiC formation as well as the recover of the IID in the Si layer.

The 3D distribution of C atoms in 8nm and 20nm SOIs was mainly analyzed by APT, where the spatial resolution is 0.5nm and the detection limit of C atoms is  $5 \times 10^{18} \text{ cm}^{-3}$  [5]. The material structures of the CSL was evaluated by CSTEM and the electron diffraction (ED) patterns obtained by fast-Fourier-transform (FFT) analysis of the lattice spots of CSTEM.  $d_S$  was evaluated by the UV-visible reflection method [1] as well as CSTEM.

PL and Raman properties of Si<sub>1-y</sub>Cy layers were measured at room temperaturre, where the excitation laser energy  $E_{EX}$  was 3.8eV and the laser diameter was 1μm. At  $E_{EX}=3.8 \text{ eV}$ , the PL photons were mainly emitted from the CSL near the SOX/Si interface, because the penetration length  $\lambda_{EX}$  of 3.8eV in Si layer is only 8nm [2]. The PL spectrum in a wide range of photon wavelengths  $\lambda_{PL}$  from the near-UV to NIR regions was calibrated using a standard illuminant [2].

## III. HCI Optimization

### A. $D_C$ Dependence of PL Property

The APT analysis for the  $Y$  depth profile of a 8-nm SOI shows that very narrow 1.5-nm-thick CSL with  $Y > 0.2$  were formed at both the SOX/Si (peak- $Y=0.25$ ) and BOX/Si (peak- $Y=0.3$ ) interfaces, just after HCI process (Fig. 1). Thus, we can detect PL emission from the CSL at the SOX/Si interface region even in a thick SOI.

The  $D_C$  dependence of PL spectrum clearly shows that the  $D_C$  of  $4 \times 10^{16} \text{ cm}^{-2}$  is the optimum dose for stronger  $I_{PL}$  (Fig. 2), which is attributable to the following mechanisms. At  $D_C \leq 4 \times 10^{16} \text{ cm}^{-2}$ ,

$I_{PL} \propto \exp(11.7Y)$  [2], because a SiC area can be formed in the CSL only at higher  $D_C$  condition. On the other hand, at  $D_C > 4 \times 10^{16} \text{ cm}^{-2}$ , the Si crystal quality is degraded with increasing  $D_C$ , resulting in the  $I_{PL}$  reduction. Hereafter, we will discuss the physical properties of a Si<sub>1-y</sub>Cy layer at the optimized  $D_C$  of  $4 \times 10^{16} \text{ cm}^{-2}$ .

### B. Material Structure: 4H-/3C-SiC Formation

The APT result in the thin SOI plane (xy plane) shows that C atoms partially cluster [6] in a low-C Si layer without CSL (inside the circles (Fig.3(a)), the cluster size is approximately 5nm. Thus, the C density fluctuates in the Si layer. As a result, the CSTEM also shows that approximately 5-nm-SiC dots, shown as moire patterns interfered by two layers of 3C-SiC and Si, were formed in Si layer (Fig.3(b)). The SiC dots with larger  $E_G$  is expected to affect the PL spectrum. Moreover, the  $Y$  fluctuates and is varied from 0.1 to 0.2 even in the surface CSL (Fig.3(c)). In the back CSL, the  $Y$  is also varied from 0.15 to 0.25. Thus, the clustered C atoms bind to Si atoms, resulting in the partial formation of SiC in CSL.

Actually, according to the CSTEM analysis of the surface CSL and the electron diffraction (ED) patterns obtained, both 4H- and 3C-SiC areas were partially formed (Figs.4), but the density of 3C-SiC,  $N_{3C}$  was higher than that of 4H-SiC,  $N_{4H}$ . However, the clear ED patterns of SiC are rarely observed, because the ED patterns in the CSL are obtained by the interference of the multiple SiC and Si layers. We also confirmed the partial formation of both 4H-/3C-SiC in the back CSL. Thus, the implanted C atoms segregate both at the SOX/Si and BOX/Si interfaces and cluster, resulting in the partial formation of both 4H-/3C-SiC areas. The surface (PL1) and back CSL (PL2) are considered to emit strong PL photons (Fig.5), and the measured PL photons in this study are mainly emitted from PL1 area, because of very small  $\lambda_{EX}$  of 8nm.

### C. $T$ Dependence of PL Property

The PL spectrum of both 8nm and 20nm Si<sub>1-y</sub>Cy layers strongly depends on the  $T$  (Figs.6 and 7). The  $I_{PL}$  increases with decreasing  $T$  in  $T \geq 700^\circ\text{C}$ , but decreases at  $T=500^\circ\text{C}$  (Fig. 7(a)). Thus, the  $T$  of about 700°C is the optimum temperature. Small  $I_{PL}$  at  $T=500^\circ\text{C}$  is attributable to the C<sup>+</sup> ion implantation induced damage in Si layer, since the FWHM of Si Raman peak increases with decreasing  $T$  (Fig. 7(b)). On the other hand, the rapid reduction of  $I_{PL}$  at  $T=1000^\circ\text{C}$  is possibly attributable to the reduction of the SiC formation at high  $T$  condition. In addition, the PL spectrum profile depends on  $d_S$  and has two peaks at  $d_S=20 \text{ nm}$  (Figs. 6), which possibly relates to the  $d_S$  dependence of  $N_{4H}/N_{3C}$  and the  $E_{PH}$  of  $\sim 3.1 \text{ eV}$  is probably the  $E_G$  of 4H-SiC [7]. Thus,  $N_{4H}/N_{3C}$  increases with decreasing  $d_S$ .

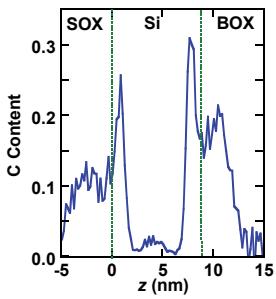
At  $d_S$  of both 8 and 20nm, PL spectrum in the whole range of  $T$  can be well fitted by two Gaussian curves of  $I_L$  with lower  $E_{PH}$  ( $E_L$ ) and  $I_H$  with higher  $E_{PH}$  ( $E_H$ ) (Figs.5, 8(a), 8(b)). Here, we compare experimental  $E_L$  and  $E_H$  with the expanded  $E_G$  of nano-dots of 3C-SiC ( $E_{3C}$ ) and 4H-SiC ( $E_{4H}$ ) [7].  $E_L$  and  $E_H$  are almost independent of  $T$  except the  $E_H$  at  $T=1000^\circ\text{C}$ , and thus the  $E_G$  of a Si<sub>1-y</sub>Cy layer is not affected by  $T$  (Fig.9(a)). It is noted that the  $E_L$  and  $E_H$  values are close to the  $E_{3C}$  and  $E_{4H}$  values, respectively. Thus, it is possible that the  $E_L$  and  $E_H$  regions of a Si<sub>1-y</sub>Cy layer are mainly composed of a 3C- and 4H-SiC nano-areas, respectively. However,  $I_L$  (3C-SiC) and  $I_H$  (4H-SiC) strongly depend on  $T$  (Fig.9(b)). Thus, the  $T$  dependence of  $I_L$  and  $I_H$  relates to that of  $N_{3C}$  and  $N_{4H}$ , respectively. Thus, the optimum  $T$  is about 700°C for forming a 3C- and 4H-SiC nano-regions in the HCI process of SOI.

## IV. Conclusion

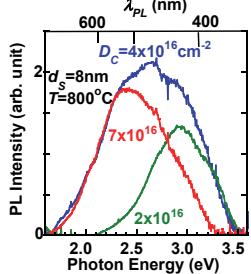
In this work, we experimentally optimized the HCI process of  $D_C$  and  $T$  in a (100) SOI substrate to form nano-SiC regions as well as to realize higher  $I_{PL}$  for a Si-based photonic device. As a result, the optimum  $D_C$  and  $T$  are about  $4 \times 10^{16} \text{ cm}^{-2}$  and  $700^\circ\text{C}$ , respectively. In addition, we experimentally confirmed the partial formation of both nano 3C- and 4H-SiC areas in the CSL at both the SOX/Si and BOX/Si interfaces.

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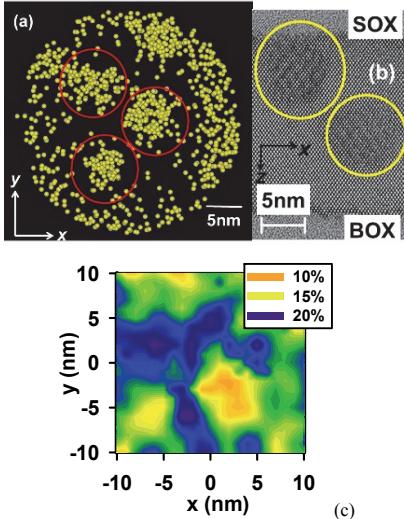
**References:** [1] T.Mizuno, JAP **55**, 04EB02, 2016. [2] T.Mizuno, JAP **56**, 04CB03, 2017. [3] T.Mizuno, JAP **50**, 010107, 2011. [4] S. Saito, IEDM 2008, Paper 19.5. [5] <http://www.nanoanalysis.co.jp/en/>. [6] Y.Shimizu, APL **98**, 232101, 2011. [7] J.Fan, *Silicon Carbide Nanostructures* (Springer), 2014.



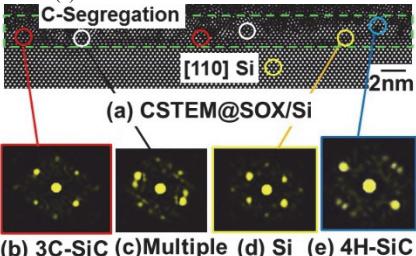
**Fig.1** APT results of non-uniform depth  $z$  profile of C content  $Y$  (solid line) in a SOI layer, where  $T=800^\circ\text{C}$ ,  $D_c=4\times 10^{16}\text{cm}^{-2}$ , and  $d_s=8\text{nm}$ .



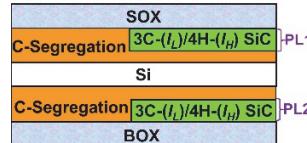
**Fig.2**  $D_c$  dependence of PL spectrum, where  $d_s=8\text{nm}$ ,  $T=800^\circ\text{C}$ , and  $E_{\text{ex}}=3.8\text{eV}$ .



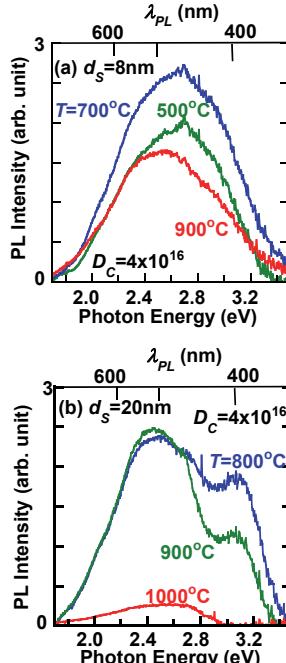
**Fig.3** APT results of C atom (yellow dots) distribution in (a) the central region of a Si layer without the CSL and (c) 2D contour maps of  $Y$  (at %) in the surface CSL, where  $T=800^\circ\text{C}$ ,  $D_c=4\times 10^{16}\text{cm}^{-2}$  and  $d_s=8\text{nm}$ . The circles in (a) show the C atom clustering (CAC). (b) CSTEM image of SiC dots inside circles in 20-nm SOI, where  $T=900^\circ\text{C}$  and  $D_c=4\times 10^{16}\text{cm}^{-2}$ . The SiC dot size in (b) is approximately 6nm, which is almost the same as that of CAC in (a).



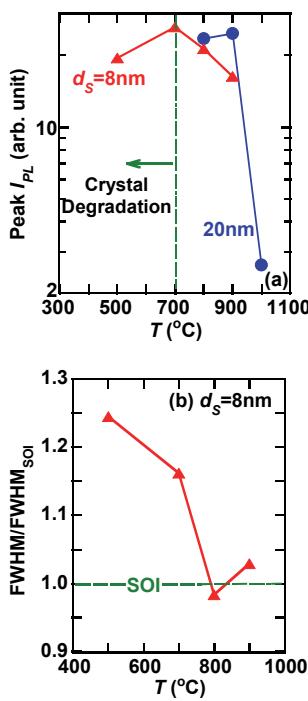
**Fig.4** (a) CSTEM image of the cross section of the surface CGL, where  $T=900^\circ\text{C}$ ,  $D_c=4\times 10^{16}\text{cm}^{-2}$  and  $d_s=8\text{nm}$ . (b) (red circles), (c) (white circles), (d) (yellow circles) and (e) (blue circle) in (a) show the ED patterns of [110]3C-SiC, multiple layers of [110]3C-SiC/Si, Si, and [2110]4H-SiC, respectively, where the diameter of all circles is approximately 2nm.



**Fig.5** Schematic cross section of SOI layers with 4H-and 3C-SiC nano-regions in the CSL near both the SOX and BOX interfaces. PL1 and PL2 show the PL emission layers at the surface and back SiC regions, respectively.  $I_L$  and  $I_H$  are PL emissions from 3C- and 4H-SiC areas, respectively. Measured PL intensity is mainly emitted from the PL1 area, because of very small  $\lambda_{\text{ex}}$  of 8nm.

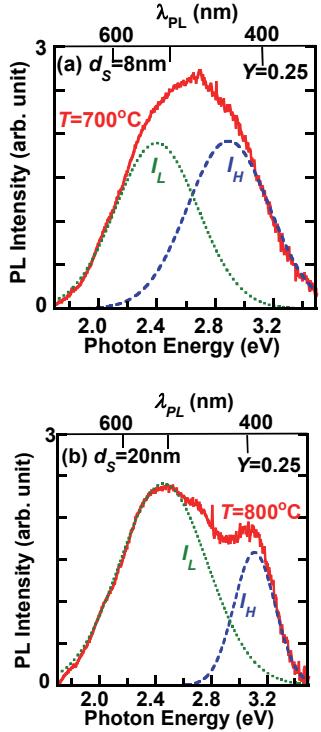


**Fig.6**  $T$  dependence of PL spectrum of  $\text{Si}_{1-x}\text{C}_y$  at (a)  $d_s=8\text{nm}$  and (b)  $20\text{nm}$ , where  $D_c=4\times 10^{16}\text{cm}^{-2}$  and  $E_{\text{ex}}=3.8\text{eV}$ . The second peak in (b) is possibly attributable to the 4H-SiC dot with higher  $E_G$  [7].

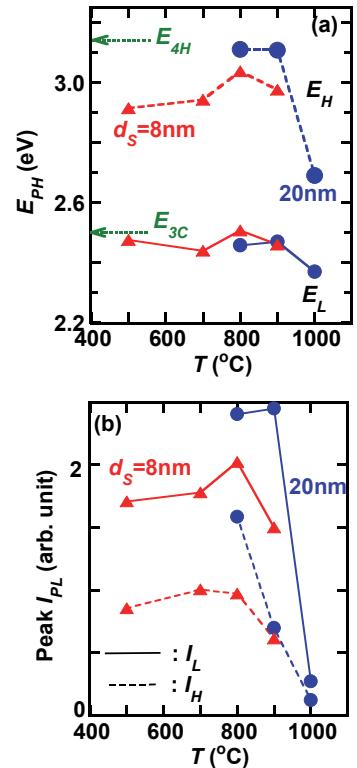


**Fig.7**  $T$  dependence of (a) peak  $I_{PL}$  and (b) FWHM of Si Raman peak at  $d_s=8\text{nm}$  normalized by that of SOI, where

$D_c=4\times 10^{16}\text{cm}^{-2}$  and  $E_{\text{ex}}=3.8\text{eV}$ . Circles and triangles in (a) show the data of  $d_s=20\text{nm}$  and 8nm, respectively.



**Fig.8** Experimental PL spectrum (solid line) of  $\text{Si}_{1-x}\text{C}_y$  layer fitted by two Gaussian curves with low ( $I_L$ : dotted line) and high  $E_{PH}$  ( $I_H$ : dashed line) at (a)  $d_s=8\text{nm}$  and (b)  $d_s=20\text{nm}$  and  $T=800^\circ\text{C}$ , where  $D_c=4\times 10^{16}\text{cm}^{-2}$ .



**Fig.9**  $T$  dependence of (a)  $E_L$  and  $E_H$ , and (b) peak- $I_L$  and  $I_H$ , where  $D_c=4\times 10^{16}\text{cm}^{-2}$ . Circles and triangles show the data at  $d_s=20\text{nm}$  and 8nm, respectively. The solid and dashed lines show the data of  $E_L$  and  $E_H$ , respectively. Arrows in (a) show the  $E_{3C}$  (~2.5eV) and  $E_{4H}$  (~3.15eV) of 2-nm SiC-dots [7].