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Two Dimensional Si-Based Semiconductor $Si_{1-Y}C_Y$: C Atom Induced Band Structure Modulation at Visible Region

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Abstract

We experimentally studied C atom impact on band structure modulation in 2D silicon carbon alloy $Si_{1-Y}C_Y$ fabricated by hot C^+ ion implantation into (100) SOI substrate in a wide range of *Y*. Photoluminescence (PL) method shows that bandgap E_G and PL intensity I_{PL} of 2D-$Si_{1-Y}C_Y$ drastically increase with increasing *Y* in high *Y* (≥0.003), and thus we demonstrated higher E_G of 2.5eV and the visible I_{PL} of wavelength λ less than 500nm. In addition, graphitic C peak at 1500cm^{-1} is also confirmed at *Y*=0.07 by UV-Raman analysis. However, even in low *Y*(<10^{-3}), I_{PL} of 2D-$Si_{1-Y}C_Y$ also increase with increasing *Y*, which is caused by the compressive strain, but *Y* dependence of E_G is very small. Thus, E_G of 2D-$Si_{1-Y}C_Y$ can be controlled by 2D-$Si_{1-Y}C_Y$ thickness d_S and *Y*.

I. Introduction

2D Si layer is a key technology for realizing extremely-thin SOIs (ETSOIs) and FinFET CMOS [1], as well as Si photonics [2]. We experimentally demonstrated phonon confinement effects (PCE) and E_G expanding due to electron confinement [3]-[5] in 2D-Si layers. A PL peak photon energy E_{PH} of a fully relaxed (100)2D-Si layer without a surface oxide [5] agrees well with theoretical E_G value [6]. Thus, E_G of (100)2D-Si can be precisely obtained by PL method.

E_G of (100)2D-Si can be controlled by d_S [5], [6], but is still lower than 1.9eV whose λ is longer than 650nm. However, to realize visible Si photonics as well as source hetero structures (SHOT) which can inject high velocity carrier into channel from high E_G source regions [7], [8], it is necessary to develop a new technology for higher E_G without controlling d_S. In 3D-$Si_{1-Y}C_Y$, E_G can increase with increasing *Y* [9]-[11], and PL intensity I_{PL} also increases with increasing *Y* [9]. Therefore, 2D-$Si_{1-Y}C_Y$ is a new candidate for E_G and λ engineering for future CMOS and Si-photonics.

In this work, we experimentally studied the impact of *Y* on E_G modulation of 2D-$Si_{1-Y}C_Y$ fabricated by $^{12}C^+$ hot ion-implantation into (100)SOIs. We obtained the *Y* dependence of E_G modulation of 2D-$Si_{1-Y}C_Y$ by PL method in a wide range of *Y* (10^{-5}<*Y*≤0.07), and demonstrated higher E_G of 2.5eV and visible λ.

II. Experiment for 2D-$Si_{1-Y}C_Y$ by Hot C^+ Implantation

High quality 2D-$Si_{1-Y}C_Y$ layers with a wide range of *Y* were fabricated by the combination of 1) $^{12}C^+$ hot ion implantation technique [12] into (100) bonded SOI substrate at higher than 900°C, and 2) two-step (low-temperature *T* after high-*T* oxidation) thermal oxidation technique [3] **(Fig.1)**. 0.5-nm thick 2D-$Si_{1-Y}C_Y$ layers with 10^{-5}<*Y*≤0.07 were successfully formed in this work.

SIMS analysis **(Fig.2)** shows that carbon density N_C in 8.5nm Si locally condenses at two interfaces of the BOX and SiO_2. However, in a d_S (≡distance between the two interfaces) limited case of 2D-Si, N_C of 2D-Si can be asuumed to be peak N_C value at the interface and uniform. Peak N_C rapidly decreases by oxidizing SOI, because of small segregation coefficients m_C of carbon at the Si/SiO_2 interface. The maximum and minimum *Y* of 0.5-nm 2D-$Si_{1-Y}C_Y$ can be estimated by SIMS analysis and Eq.(1) (Fig.3 caption), and be achieved to be about 0.07 and 10^{-5}, respectively, using various $^{12}C^+$ dose ($5\times10^{12}\leq D_C\leq 2\times10^{16}$cm^{-2}).

We analyzed the E_G properties of 0.5nm thick 2D-$Si_{1-Y}C_Y$ layers evaluated by PL method, where excitation laser energy $h\nu$ was varied from 2.3 to 3.8eV at room temperature [3]. Laser power P_L was set to be 1mW to compress the P_L heating of Si [3], and the laser diameter was 1μm. Phonon properties of 2D-$Si_{1-Y}C_Y$ layers were measured by UV (325-nm)/visual (532-nm) Raman spectroscopy. We observe no degradation of the FWHM of Si peak even at D_C= 2×10^{16} cm^{-2}, which is the benefit of hot C^+ implantation technique.

III. Large E_G Modulation by C Atom

A. PL Si-C Peak in 2D-$Si_{1-Y}C_Y$

UV-Raman analysis shows double peaks of D and G bands of graphitic C at about 1500cm^{-1} [11] **(Fig.3)** only in *Y*=0.07, and thus silicon-carbon alloys were successfully fabricated.

Very large and double-peak PL spectra excited by 2.3eV laser can be newly observed at *Y*≥0.003 **(Fig.4)**. The lower E_{PH} peak is attributable to 2D-Si [3], but new higher E_{PH} is considered to be PL from the 2D Si-C alloy. I_{PL} of both Si and Si-C peaks drastically increases with increasing *Y* **(Figs.4, 5)** in *Y*≥0.003, compared to I_{PL} at *Y*=0; I_{PL0}, resulting in $I_{PL}/I_{PL0} \propto Y^{1.4}$ (**2**) **(Fig.5)**. Especially, I_{PL}/I_{PL0} at *Y*=0.07 reaches over 20, which is very suitable for Si photonics. Here, $I_{PL} \propto \alpha\eta = \alpha/(1+\tau_R/\tau_{NR})$ (**3**) , where α, η, τ_R, and τ_{NR} are absorption coefficient, luminescence efficiency, radiative, and non-radiative life times of electrons, respectively [15]. Thus, when η=const., α of 2D-$Si_{1-Y}C_Y$; α_{SC} is estimated to be about 26 times as large as that of 2D-Si (α_{2D}) which is also two orders of magnitude larger than that of 3D-Si (α_{3D}) [14], resulting in $\alpha_{SC}/\alpha_{3D}\approx3300$ **(Fig.5)**. However, the I_{PL} at $Y\approx3\times10^{-3}$ has the minimum value **(Fig.5)**, which is possibly due to the τ_{NR} decrease with increasing *Y*, because of C^+ ion damage.

Moreover, PL spectrum of 2D-$Si_{0.93}C_{0.07}$ in visible region strongly depends on $h\nu$ **(Fig.6)**, because electrons cannot be generated by lower $h\nu$ (E_G>$h\nu$). When $h\nu$=3.8eV, we can newly observe visible PL spectrum. The peak E_{PH} reaches 2.5eV, resulting in peak-$\lambda\approx$500nm. PL spectrum tail can be also detected even in higher than 3eV. However, since the PL peak was very broad in *Y*<0.07, E_G of 2D-$Si_{1-Y}C_Y$ is almost independent of *Y*, but is higher than E_G of 3D-$Si_{1-Y}C_Y$ [9] **(Fig.7)**. Consequently, 2D-$Si_{1-Y}C_Y$ with high *Y* is a very promising for visible Si-photonics and SHOT.

B. PL Si-Peak in 2D-$Si_{1-Y}C_Y$

Even when $Y=4\times10^{-4}$, we can observe I_{PL} enhancement (I_{PL}/I_{PL0}=1.66) and E_G expanding (=1.8eV) **(Fig.8)**. However, no PL Si-C peak was observed in Y<0.001 **(Fig.8)**. Lattice constant 2D-$Si_{1-Y}C_Y$ a_{SC} also decreases with increasing *Y*, compared with that of 2D-Si a_S [11]. Thus, the compressive strain ε_C in 2D-$Si_{1-Y}C_Y$ increases with increasing *Y* **(Fig.9)**, according to ε_C formula of 3D-$Si_{1-Y}C_Y$ [11];$\varepsilon_C(Y) = (a_S - a_{SC}(Y))/a_S = (-0.24Y + 0.057Y^2)/a_S$ (**4**). So, residual tensile strain $\varepsilon_T(Y)$ of 2D-Si, which is applied by the large difference of expansion coefficient between SiO_2 and 2D-Si [5], can be relaxed by the equations of Eq.(4) and $\varepsilon_T(Y) = \varepsilon_{T0} - \varepsilon_C(Y)$ (**5**) (ε_{T0} is the residual tensile strain (0.33%) in 0.5-nm 2D-Si) **(Fig.9)** without etching SiO_2. Thus, using $E_G(Y) \propto \exp\left(\left(\varepsilon_{T0} - \varepsilon_C(Y)\right)/\varepsilon_0\right)$ (**6**), where ε_0 the fitting parameter (0.22%) [5], E_G rapidly increases with increasing *Y* even in *Y*<10^{-3} **(Fig.10)**, which can be well explained by the ε_T relaxation induced E_G expansion by Eq.(6). Thus, even small *Y* (<10^{-3}) can affect the band structure of 2D-$Si_{1-Y}C_Y$.

C. Device Design for High E_G and Visible Photon Emission

According to the above discussions and our previous works [4], [5], it is possible to control higher E_G and shorter photon emission of 2D Si-based semiconductor, by designing only three key parameters of d_S, SiO_2 thickness T_{OX}, and *Y*. For example, when d_S≥0.5nm **(Fig.11)**, thinner d_S in 2D-Si is required to realize band structures with 1.1<E_G≤2.1eV or λ≥600nm [4]. Especially in the case of 1.7<E_G≤2.1eV, the 2D-Si must be relaxed by thinning T_{OX} [5]. In addition, to realize E_G>2.1eV (λ<600nm), a 2D silicon-carbon alloy technology is strongly necessary.

IV. Conclusion

We experimentally studied C content effects on band structure modulation in a 0.5-nm 2D-$Si_{1-Y}C_Y$ layer fabricated by C^+ hot ion implantation technique into (100)SOI. PL can be detected in a wide range of 10^{-5}<*Y*≤0.07. I_{PL} and E_G of 2D-$Si_{1-Y}C_Y$ rapidly increases with increasing *Y*, and E_G of 2.5eV and visible λ of 500-nm can be achieved at *Y*=0.07. Consequently, we can precisely design a future 2D device with various high-E_G and visible λ, by controlling only three parameters of d_S, T_{OX}, and *Y*.

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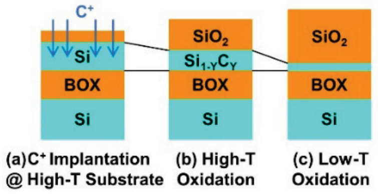

Fig.1 Schematic fabrication for 2D-$Si_{1-Y}C_Y$ layers. (a) After $^{12}C^+$ implantation into 1000ºC (100)SOI substrate, (b) Si was thinned by 1000°C oxidation. D_C was varied from 5×10^{12} to 2×10^{16}cm^{-2}. (c) Additional 900°C oxidation was carried out to form 0.5nm-region thick $Si_{1-Y}C_Y$ layer, resulting in $10^{-5}\leq Y\leq 0.07$.

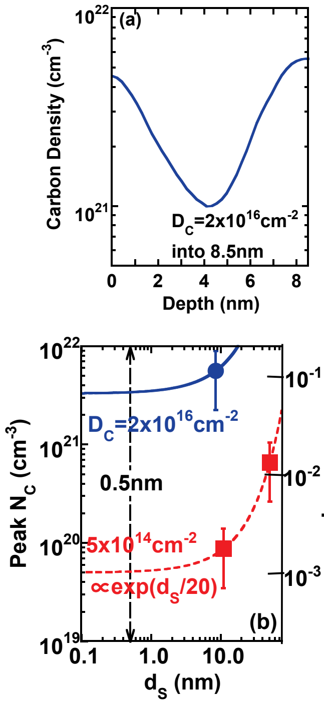

Fig.2 (a) SIMS (solid line) results of N_C (dashed line) just after hot C^+ ion implantation into 8.5-nm SOI which is the minimum thickness for SIMS, where D_C is 2×10^{16}cm^{-2}. (b) Experimental peak N_C at the Si/BOX interface with error bars (about 60%) due to SIMS accuracy which is very low at the interface, where D_C=2×10^{16} (circle) and 5×10^{14}cm^{-2} (triangles). N_C decreases with oxidizing Si, because of the small m_C at SiO_2/Si. d_S dependence of $N_C(d_S)$ can be obtained by the following 1D-differential equation: $dN_C/dx \propto N_C(x)$ resulting in $N_C(d_S) = N_0 \exp(d_S/d_0)$ **(1)** (solid line), where N_0 which depends on D_C and fitting d_0 (=20nm) is constant. Solid and dashed lines show the estimated d_S dependence of peak N_C by Eq.(1). As a result, the right axis shows that the maximum Y was 0.07 at d_S=0.5nm.

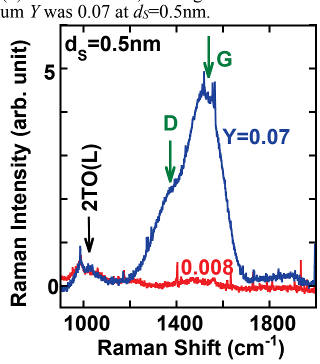

Fig.3 UV-Raman spectra at Y of 0.07 (blue line) and 0.008 (red line), where d_S=0.5nm. Double Raman peaks at Y=0.07 are attributable to D (1340cm^{-1}) and G (1500cm^{-1}) bands of graphitic C [11], whereas low Y sample shows no C band. Raman peak at about 1000cm^{-1} shows the phonon mode of Si 2TO(L) [13].

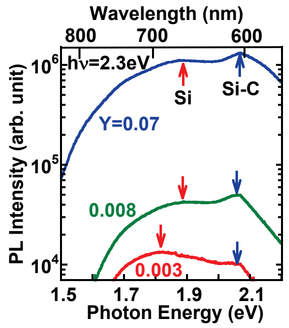

Fig.4 PL spectra excited by 2.3eV laser as a function of Y at Y≥0.003 condition, where d_S=0.5nm. Lower and upper axes show PL photon energy and wavelength, respectively. Arrows show peak I_{PL} which are attributable to Si and Si-C alloy.

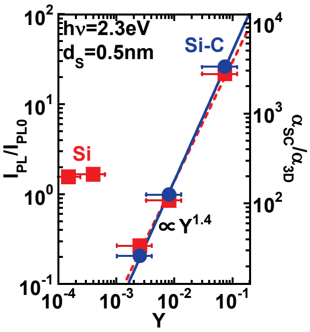

Fig.5 Peak I_{PL} of 2D-$Si_{1-Y}C_Y$ normalized by that of 2D-Si; I_{PL0} vs. Y, where $h\nu$=2.3eV and d_S=0.5nm. The right axis shows the estimated α_{SC} of 2D-$Si_{1-Y}C_Y$ normalized by α_{3D} of 3D-Si. Circles and squares show Si-C and Si peaks, respectively. Solid and dashed lines shows the fitting curves of $I_{PL} \propto Y^{1.4}$ in Y>10^{-3}, where the correlation coefficient was about 1. Error bars show the Y accuracy (60%) obtained by SIMS.

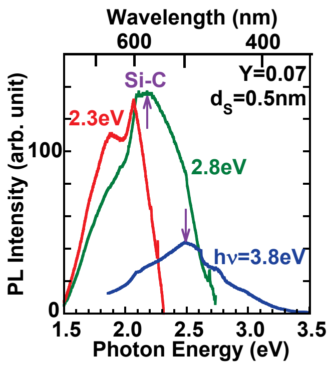

Fig.6 Excitation laser energy dependence of PL spectra at Y=0.07 in visible region, where d_S=0.5nm. Blue, green, and red lines show the data excited by $h\nu$ of 3.8, 2.8, and 2.3eV, respectively.

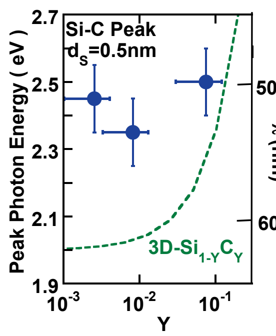

Fig.7 Y dependence of E_G (left axis) and λ (right axis) at Si-C peak (circles), where $h\nu$=3.8eV and d_S=0.5nm. Dashed line shows the data of 3D-$Si_{1-Y}C_Y$ [9].

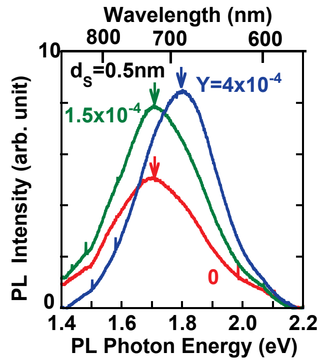

Fig.8 PL spectra as a function of Y in low Y condition ($\leq 4\times10^{-4}$), where $h\nu$=2.3eV and d_S=0.5nm. I_{PL} also increases with increasing Y, and E_G at Y=4×10^{-4} increases even at Y<0.1%.

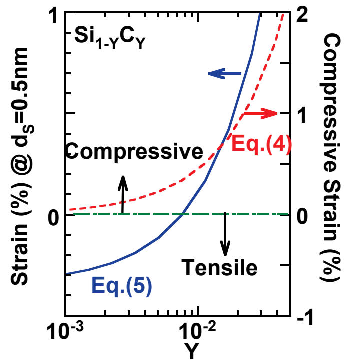

Fig.9 Y dependence of estimated strain (solid line) of 0.5nm $Si_{1-Y}C_Y$ by Eq.(5) and calculated compressive-strain (dashed line) of 3D-$Si_{1-Y}C_Y$ [11] by Eq.(4).

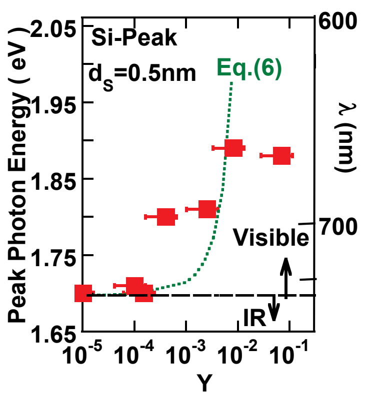

Fig.10 Y dependence of E_G (left axis) and λ (right axis) at peak I_{PL} of Si (squares), where $h\nu$=2.3eV and d_S=0.5nm. Dotted lines shows the tensile strain dependence of E_G model in 2D-$Si_{1-Y}C_Y$ by Eq.(6).

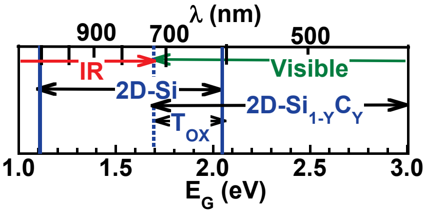

Fig.11 Device design for realizing higher E_G and visible λ in 2D-$Si_{1-Y}C_Y$ and 2D-Si, where d_S≥0.5nm. Lower and upper axes show E_G and λ, respectively. There are only three key parameters of d_S, T_{OX}, and Y for realizing various E_G in 2D-Si device.