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Surface-Orientation/Strain Dependence of Quantum Confinement Effects in Si Monolayers for Future CMOS Devices

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I. Introduction

Two dimensional (2D) Si structures are widely used for extremely-thin SOI (ETSOIs) and FinFET CMOS [1], as well as Si photonic devices [2]. In addition, surface orientation engineering, such as (110) Si for p-MOS, and strain technique have been widely studied for realizing a high speed CMOS [3]. To improve short channel effects (SCE) of CMOS and photoluminescence (PL) intensity of Si photonic devices, the 2D-Si thickness T_S is required to continue decreasing. It is reported that in low-D Si-nanostructures (Si nanowires (1D) and nanocrystals (0D)) [3], quantum mechanical confinements (QMC), including phonon confinement effects (PCE) due to the uncertainty principle in a nanometer size, are enhanced. The PCE induces the carrier mobility reduction due to the enlarged phonon scattering of carriers [3]. Recently, we have experimentally demonstrated the PCE even in a (100) 2D-Si monolayer with $T_S \approx a_S$ (Si lattice constant) [4]. However, other physical properties of Si monolayer structures have not been studied in detail, yet.

In this work, we have experimentally studied the surface orientation and the tensile strain effects on both the PCE and the PL results of the 2D-Si monolayers with the minimum $T_S \approx a_S/2$. We have shown the enhancement of both the PCE and the PL intensity at T_S<1nm, and also discussed physical properties of 2D-Si, such as the carrier saturation velocity v_{SAT}, and the bandgap E_G.

II. Experimental for Various 2D-Si Layers

2D-Si was fabricated by thermal oxidation processes of bonded (100)SOI, (110)SOI, and (100)SSOI substrates ar high temperature T (1000°C), where their initial T_S is several ten nm, and the initial biaxial strain value of SSOIs is 0.7%. Therefore, the three substrates have SiO_2/Si/BOX (buried oxide) quantum well structures, where the thicknesses for the SiO_2 and the BOX are about 100 and 150nm, respectively.

The T_S of 2D-Si layers is mainly evaluated by UV/visual reflection spectrum [4], which is also verified by HRTEM. We have measured the PCE by a UV (325 nm) Raman spectroscopy and the PL as a function of an excitation laser photon energy $h\nu$ (h is Planck constant and ν is photon frequency) of 2.33 (532 nm), 2.81 (441 nm), and 3.81 eV (325nm) at room temperature, where the laser power is 1 mW, the laser diameter is 1 μm, and the laser penetration length λ_P of 532, 441, and 325 nm in the 3D-Si layer are about 1000, 500, and 5 nm, respectively.

III. Phonon Confinement Effects

According to UV-Raman spectroscopy I_R of (100)SOI, (110)SOI, and (100)SSOI (Figs. 1(a)-(c)), when T_S<5 nm, we have observed the asymmetric broadening and the peak-downshift $\Delta\omega$ from a usual 3D-Si peak (520cm^{-1}) in all Si substrates. The $\Delta\omega$ is attributable to the decrease of optical phonon energy E_P in 2D-Si layers, because the force constant α_F decreases in a 2D-Si lattice, compared to the α_F in a 3D-Si [6]. The PCE is enhanced with decreasing T_S, and becomes very large especially in 0.25nm (100)SOI. Thus, for the first time, we have verified the PCE even in (110)SOI and SSOI.

The asymmetric broadening, defined by full width at tenth maximum (FWTM) of the Raman peak, has a strong T_S dependence (Fig.2). The FWTM of 2D-Si rapidly increases with decreasing T_S, but is independent of the surface orientation. However, the FWTM is enhanced by the tensile strain. Moreover, the Raman peak intensity I_P in 2D-Si increases with decreasing T_S, which is due to the resonance Raman scattering. Thus, the Si intensity under the BOX can be neglected, compared to the I_P of 2D-Si.

The $\Delta\omega$ rapidly increases with decreasing T_S in all Si substrates (Fig.3), which is also due to the PCE. Subtracting the $\Delta\omega$ caused by only PCE from SSOI data, the strain value can keep almost constant (0.7%) at T_S>2nm, but drastically increases at T_S<1nm, which is probably caused by the tensile strain in the Si/SiO_2 interface affected by thermal stress of SiO_2 into the Si layer [5].

Most E_P values of 2D-Si layers are lower than 64meV of 3D-Si [6] (Fig.1). Assuming that the E_P of 2D-Si has almost the same distribution function of $I_R(E_P)$, the v_{SAT} of the 2D-Si layer can be estimated, using $v_{SAT} \propto E_P^{1/2}$ [6]. Thus, the v_{SAT} of the 2D-Si is reduced by the lower E_P. Fig.4 shows the T_S dependence of an average v_{SAT} calculated by $v_{SAT} \propto \int E_P^{1/2} I_R(E_P) dE_P / \int I_R(E_P) dE_P$. The average v_{SAT} rapidly decreases at T_S<1nm, and is reduced by 5% at T_S=0.25nm, which is also the physical limitation of the 2D-Si layer.

IV. Photoluminescence from 2D-Si Layer

It is expected that PL characteristics strongly depend on the Si surface orientation, because only (100) 2D-Si layer is considered to be a direct bandgap structure [2]. Fig. 5(a) shows PL spectra of (100) and (110)SOIs at room T as a function of $h\nu$, where $T_S \approx$0.5nm. When $h\nu \le$2.81eV, the PL spectrum shows very broad (FWHM≈0.3eV), similar to those of Si photonics [2] and porous Si [3], and is independent of $h\nu$. However, the PL spectrum at $h\nu$=3.81 shows very sharp (FWHM≈0.013eV), and the peak photon energy E_{PH} is higher than E_{PH} at $h\nu \le$2.81eV. On the other hand, we cannot detect the PL spectrum from the (110)SOI, which is probably due to the fact that optical transition in (110)SOI with $T_S \approx$0.5nm is still indirect [2]. Moreover, Fig. 5(b) shows that both the E_{PH} and the PL intensity I_{PL} of (100)SOI at $h\nu$=2.33eV strongly depend on the T_S. The I_{PL} at $h\nu$=2.33eV of only (100)SOI rapidly increases with decreasing T_S (Fig.6), but the I_{PL} also decreases at $T_S \approx$0.25nm. Here, when $T_S \ge$0.5nm, I_{PL} is considered to be proportional to the excitation laser photon flux I_{FA} absorbed in 2D-Si with T_S, and thus $I_{FA} \propto [1-\exp(-T_S/\lambda_P)]$. As a result, the λ_P of (100) 2D-Si (dashed line) rapidly decreases with decreasing T_S. Very short λ_P and high I_{PL} are very suitable for a photonic device, which indicates the optical direct-transitions in (100) 2D-Si, because the λ_P is reduced in the case of the direct transitions [6].

Moreover, the E_{PH} at $h\nu$=2.33eV expands with decreasing T_S and is independent of the strain (Fig.7). The E_{PH} values are smaller than the theoretical QCE results of E_G values [7], which may be due to the exciton levels beneath the conduction band level [6]. Thus, it is suggested that E_G of 2D-Si layer expands with decreasing T_S. However, the E_{PH} at $h\nu$=3.81eV is independent of the T_S [4]. Thus, the PL characteristics at $h\nu \le$2.81eV is much different from those at $h\nu$=3.81eV, which indicates that the PL strongly depends on ($h\nu - E_\Gamma$), where E_Γ (~2eV) is the direct bandgap energy at Γ point of (100) 2D-Si [2].

To explain the above PL results, we have introduced PL models. When $h\nu \gg E_\Gamma$ (Fig.8(a)), generated hot electrons can be injected into the E_G transition region in SiO_2/Si interface [8], and the photon emission occurs by the recombination of electron/hole pairs. Therefore, the E_{PH} at $h\nu$=3.81eV is proportional to ($E_I - E_V$) and thus is independent of the E_G of 2D-Si, where E_I and E_V are interface state and the valence band levels, respectively. On the other hand, when $h\nu \approx E_\Gamma$ (Fig.8(b)), generated electron/hole pairs are recombined in the 2D-Si region with direct bandgap, and thus the E_{PH} strongly depends on the $E_G(T_S)$ of 2D-Si.

V. Conclusion

We have experimentally studied the surface orientation/strain effects on quantum mechanical confinements (QMC) in 2D-Si layers for future CMOS/Si photonics devices. Using UV-Raman spectroscopy, we have demonstrated that quantum phonon confinement effects (PCE) strongly depends on the 2D-Si thickness T_S, but is independent of the surface orientation. The PCE is also enhanced by the strain. Thus, carrier saturation velocity is reduced by the lower phonon energy due to PCE. On the other hand, photoluminescence (PL) properties, emitted from only (100) 2D-Si layers, depends on the excitation photon energy $h\nu$ (2.33≤$h\nu$≤3.81eV), and the PL intensity increases with decreasing T_S. The PL data can be explained by the simple PL models considering band modulation. Consequently, it is necessary to reconstruct the device design for the 2D-Si CMOS, but the (100) 2D-Si structure is very promising for future Si photonic devices.

References: [1] A. Nazarov, *SOI Materials for Nanoelectronics Applications*, (Springer) 2011. [2] S. Saito, IEDM 2008, Paper 19.5. [3] V. Kumar, *Nanosilicon*, (Elsevier), 2008. [4] T. Mizuno, Jpn. J. Appl. Phys. **51** (2012) 02BC03. [5] Y. Takahashi, Jpn. J. Appl. Phys. **34** (1995) 950. [6] S. M. Sze, *Physics of Semiconductor Devices* (Wiley), 1981. [7] B. K. Agrawal, Appl. Phys. Lett. **77** (2000) 3039. [8] Y. Yamashita, Phys. Rev. **B73** (2006) 045336.

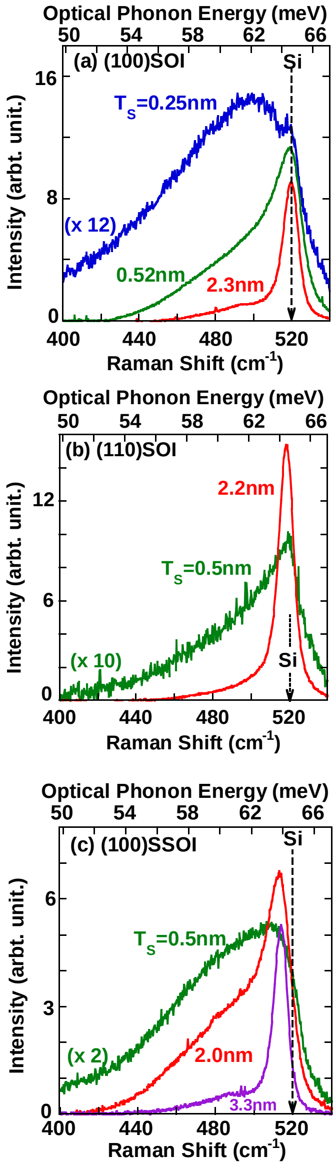


Fig.1 UV Raman spectra of (a) (100)SOI, (b) (110)SOI, and (c) (100)SSOI substrates in various 2D-Si thickness T_S. Upper and lower axes show optical phonon energy E_P ($\equiv hc\omega$) and wave number ω, respectively, where c is speed of light and ω is Raman wave number. Asymmetrical broadening and peak-shift of Raman shift increases with decreasing T_S in all substrates.

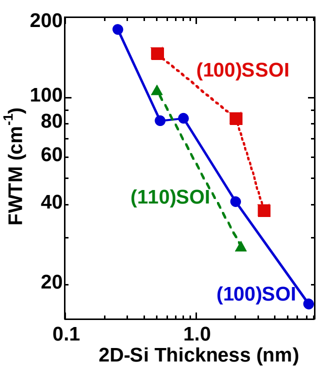


Fig.2 T_S dependence of FWTM (Full Width at Tenth Maximum) of the Raman peak of (100)SOI (circles), (110)SOI (triangles), and (100)SSOI (squares). FWTM values of (100) and (110) 2D-Si layers increase with decreasing T_S and are proportional to $T_S^{-0.7}$. In addition, the FWTM values are enhanced by the strain in (100)SSOIs.

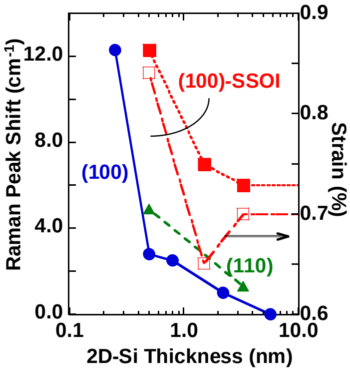


Fig.3 T_S dependence of $\Delta\omega$ of (100)SOI (circles), (110)SOI (triangles), and (100)SSOI (squares). The $\Delta\omega$ value increases with decreasing T_S in all substrates. Right vertical axis shows the tensile strain values (open squares) of (100)SSOIs and the strain rapidly increases at T_S≤1nm .

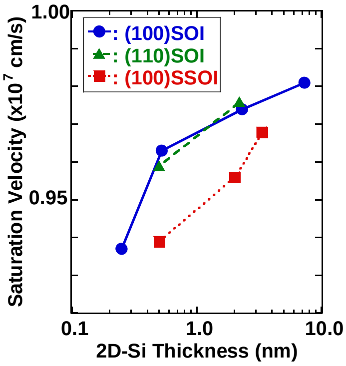


Fig.4 T_S dependence of the average v_{SAT} values of (100)SOI (circles), (110)SOI (triangles), and (100)SSOI (squares), using $v_{SAT}\propto E_P^{1/2}$. The v_{SAT} rapidly decreases, when T_S≤1nm.

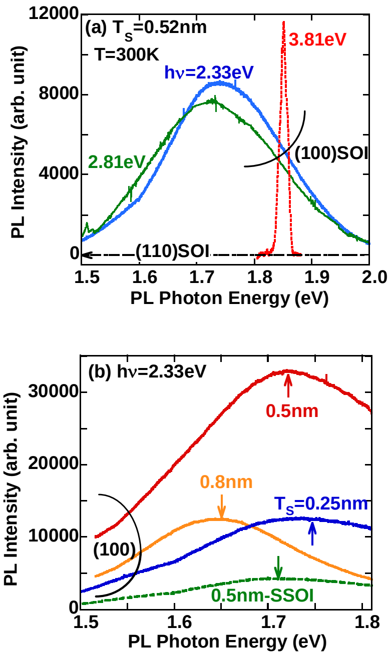


Fig.5 (a) $h\nu$ dependence of PL spectra vs. PL photon energy of (100) and (110) SOIs at T_S≈0.5nm, where 2.33≤$h\nu$≤3.81eV. We cannot detect the PL intensity of (110)SOIs. The PL shows very sharp only at $h\nu$=3.81eV. (b) T_S dependence of PL spectra vs. PL photon energy of (100)SOI (solid lines) and (100)SSOI (dashed line), and the arrows show the peak E_{PH} in various T_S, where 0.25≤T_S≤0.8nm. Lattice temperature T is 300K.

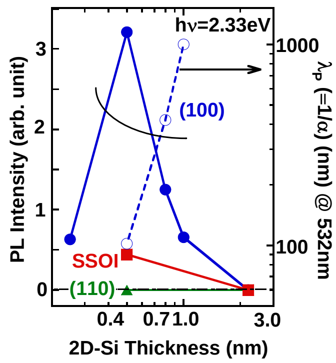


Fig.6 PL intensity of (100)SOI (circles), (110)SOI (triangles), and (100)SSOI (squares) as a function of T_S, where T is 300K and $h\nu$=2.33eV. I_{PL} of (100)SOI rapidly increases at T_S≤1nm, but also decreases at T_S=0.25nm. Moreover, I_{PL} of (100)SSOI is very weak. Right vertical axis shows estimated λ_P (≡1/α (α is the absorption coefficient)) of (100)SOI (open circles) at $h\nu$=2.33eV, and the dashed line indicates that $\lambda_P\propto T_S^{3.2}$.

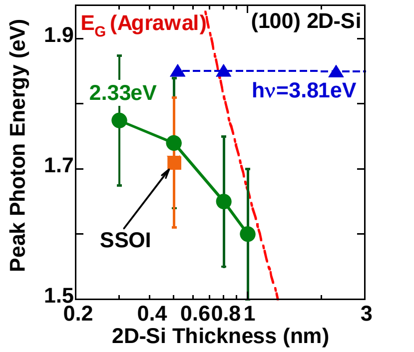
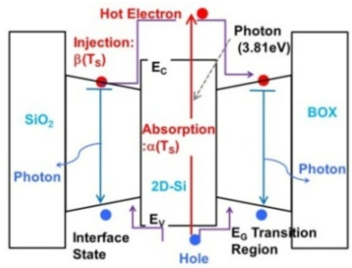
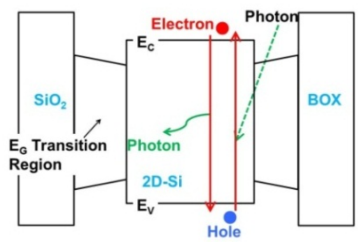


Fig.7 T_S dependence of PL peak photon energy at T=300K. Circles and triangles show the results of (100)SOI at $h\nu$=2.33eV and 3.81eV, respectively. Square show the result of (100)SSOI at $h\nu$=2.33eV. Error bars show the standard deviation of E_{PH} (0.1eV). The dotted/dashed line shows theoretical T_S dependence of E_G values of (100) 2D-Si [7]. The E_{PH} only at $h\nu$=2.33eV increases with decreasing T_S.



(a) $h\nu$=3.81eV>>E_Γ



(b) $h\nu$=2.33/2.81eV≈E_Γ

Fig.8 PL models for 2D-Si layers. (a) When $h\nu$=3.81eV>>E_Γ (E_Γ (~2eV) [2] is the direct bandgap energy at Γ point of (100)2D-Si.), generated hot electron/hole pairs recombine in the Si/SiO$_2$ interface of three-region model [5], where α(T_S) and β(T_S) are the absorption coefficient of photons and the injection coefficient of hot electrons into the interfaces, respectively. (b) When $h\nu$=2.33/2.81eV≈E_Γ, electron/hole pairs directly recombine in a 2D-Si layer with direct bandgap.