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)-SOI, and photonic structure 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 saturation velocity $v_{SAT}$ and the bandgap $E_G$.

Recent measurement of 2D-Si quantum properties by Raman spectroscopy [4] and absorption spectroscopy [5] demonstrated that a 2D-Si layer is a good candidate for future electronic devices and photonic devices. 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 $T_S$ of 2.81 (441 nm), and 3.81 eV (325nm) at room temperature, where the laser power is 1 mW, the laser diameter is 1<sub>nm</sub>, 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)SOI substrates at high temperature $T$ (1000°C), where their initial $T_S$ is several ten nm, and the initial biaxial strain of SOIs is 0.7%. Therefore, where substrates have SiO$_2$/Si BOX (buried) 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 $h\nu$, where $h\nu=2.33$ (532 nm), and 3.81 eV (325nm) at room temperature, where the laser power is 1 mW, the laser diameter is 1<sub>nm</sub>, and also discussed physical properties of 2D-Si, such as the carrier saturation velocity $v_{SAT}$ and the bandgap $E_G$.

III. Phonon Confinement Effects

According to UV Raman spectroscopy $I_\omega$ of (100)SOI, (110)SOI, and (100)SSOI substrates (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 at 520 cm$^{-1}$ 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 $\alpha_F$ decreases in a 2D-Si lattice, compared to the $\alpha_F$ 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 $I_R$ 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 $I_R$ of 2D-Si. The $\Delta\omega$ rapidly increases with decreasing $T_S$ in all substrates (Fig.3), which is also due to the PCE. Substracting the $\Delta\omega$ caused by only PCE from SSOI data, the strain value can keep almost constant (0.7%) at $T_S=2$nm, but drastically increases at $T_S=1$nm, which is partly caused by the dehiscence strain, and the Si/SSO$_2$ 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 $I_\omega(E_P)$, 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 $\langle I_\omega/E_P \rangle$ (Fig.3(b)). The average $v_{SAT}$ rapidly decreases at $T_S<1$nm, and is reduced by 5% at $T_S=0.25$nm, 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 of the direct bandgap layer band [3]. However, the PL intensity in the 2D-Si is strongly dependent on the 2D-Si thickness $T_S$ at $h\nu=3.81$eV. Moreover, the $T_S$ dependence of (100)2D-Si (dashed line) rapidly decreases with decreasing $T_S$. Very short $\lambda_P$ and high $I_P$ are suitable for a photonic device, which indicates the optical direct-transitions in (100) 2D-Si, because the $\lambda_P$ is reduced in the case of the direct transitions [6].

Moreover, the $E_P$ at $h\nu=3.23$eV expands with decreasing $T_S$ and is independent of the strain (Fig.7). The $E_P$ values are smaller than the theoretical QCE results of $E_P$ values [7], which may be due to the excitation levels (100) layers. However, the PL spectrum at $h\nu=3.81$eV is independent of the $T_S$ [4]. Thus, the PL characteristics at $h\nu=3.23$eV is much different from those at $h\nu=3.81$eV, which indicates that the PL strongly depends on $h\nu$. Moreover, the $\lambda_P$ decreases with decreasing $T_S$. In this case, the $T_S$ dependence of the PL on $h\nu$ at $h\nu=3.81$eV is considered to be a direct bandgap layer at $T_S$ point of (100)2D-Si [2].

We have experimentally studied the surface orientation/strain effects on quantum mechanical confinements (QMC) in 2D-Si layers for future CMOS/Si photonic devices. Using UV-Raman spectroscopy, we have demonstrated that quantum phonon confinement effects (PCE) strongly depend on the 2D-Si thickness $T_S$, but is independent of the surface orientation. The PCE is also enhanced by the strain. Carrier saturation velocity $v_{SAT}$ 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<sub>nm</sub>) and the PL intensity increases with decreasing $T_S$. The PL data in all Si thickness dependence of $\alpha_F$ are recombined in the 2D-Si region with direct bandgap, and thus the $E_P$ strongly depends on the $E_P$ of 2D-Si ($T_S$). V. Conclusion
increases with decreasing \( T_s \). Asymmetrical broadening and peak-shift of Raman shift speed of light and \( T_s \). (c) (100)SSOI substrates in various 2D-Si thickness \( T_s \) and (1) (100)SSOI substrates in various 2D-Si thickness \( T_s \). Upper and lower axes show optical phonon energy \( \hbar \omega \) and wave number \( \omega \) respectively. Where \( \omega \) is speed of light and \( \omega \) is Raman wave number. Asymmetrical broadening and peak-shift of Raman shift increases with decreasing \( T_s \) in all substrates.

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)SSOI and the strain rapidly increases at \( T_s \leq 0.2 \text{nm} \). The dotted/dashed line shows theoretical \( \Delta \omega \) dependence of \( T_s \). The error bars show the average value of three regions, where \( \Delta \omega \) rapidly increases at \( T_s < 0.2 \text{nm} \). Moreover, the PL model for (100)SSOI in very weak. 

Fig.4 \( T_s \) dependence of the average \( v_{SAT} \) values of (100)SOI (open circles), (110)SOI (triangles), and (100)SSOI (squares), using \( \gamma \). The \( v_{SAT} \) rapidly decreases, when \( T_s \leq 0.2 \text{nm} \).

Fig.5 (a) \( h \nu \) dependence of PL spectra vs. PL photon energy of (100) and (110) SOIs at \( T_s \geq 0.5 \text{nm} \), where \( 2.33 \text{eV} \leq h \nu \leq 3.81 \text{eV} \). The PL intensities of (100)SOI and (110)SOI are shown by open circles and solid line, respectively, where \( \alpha \) is absorption coefficient of photons and \( T_s \) is temperature. Error bars show the standard deviation of \( E_{PH} \) at \( 0.1 \text{eV} \). The dotted/dashed line shows the theoretical \( T_s \) dependence of \( E_{PH} \) values of (100) 2D-Si [7]. The \( E_{PH} \) only at \( h \nu = 2.33 \text{eV} \) increases with decreasing \( T_s \).

Fig.6 PL intensity of (100)SOI (circles), (110)SOI (triangles), and (100)SSOI (squares) as a function of \( T_s \) where \( T_s \) is 300K and \( h \nu = 2.33 \text{eV} \). The PL intensity of (100)SOI rapidly increases at \( T_s \leq 0.1 \text{nm} \) but also decreases at \( T_s \geq 0.2 \text{nm} \). Moreover, the PL intensity of (100)SSOI is very weak. The dotted/dashed line indicates that \( \Delta \omega \leq T_s \).

Fig.7 \( T_s \) dependence of PL peak photon energy at \( T_s = 300 \text{K} \). Circles and triangles show the results of (100)SOI at \( h \nu = 2.33 \text{eV} \) and \( 3.81 \text{eV} \), respectively, where \( \Delta \omega \) is the rayout from the value of (100)SOI at \( h \nu = 2.33 \text{eV} \). The dotted/dashed line shows theoretical \( T_s \) dependence of \( E_{PH} \) only at \( h \nu = 3.81 \text{eV} \) increases with decreasing \( T_s \).