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Impact of Surface Oxide Layer on Band Structure Modulation in Si Quantum Well Structures

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Abstract

We experimentally studied an impact of the surface oxide layer on quantum confinement effects (QCE) in surface-oxide/two dimensional (2D)-Si/BOX (buried oxide) quantum well structures (SQW), using UV-Raman spectroscopy, photoluminescence (PL) method, and 2D stress simulator. UV-Raman data show that tensile strain of SQW, stressed by a thermal expansion mismatch between oxide and Si layers, decreases with decreasing the surface oxide thickness T_{OX}. According to the strain behavior in SQW and strained-Si, PL results show that bandgap E_G of the SQW rapidly expands with decreasing T_{OX}. However, QCE in SQW keep stable in spite of high temperature postannealing process.

I. Introduction

We experimentally demonstrated phonon confinement effects (PCE) and bandgap (E_G) expanding due to electron confinement [3]-[5] in 2D Si layers, which are key structures for realizing extremely-thin SOIs (ETSOIs) and FinFET CMOS [1], as well as Si photonic devices [2]. In a SQW, the 2D-Si layer is stressed by a thermal expansion/contraction mismatch between 2D-Si and surface oxide layers [6]-[7], because the linear coefficient of thermal expansion of Si; α_S is about 5 times as large as that of oxide; α_{OX} [8]. In addition, it is reported [9] that Young's modulus E of 2D-Si rapidly decreases with decreasing the 2D-Si thickness T_S. The oxide stress effect on 2D-Si performance is considered to be enhanced with decreasing T_S. Therefore, it is very important to clarify the oxide layer influence on the physical properties of 2D-Si, and thus to study an intrinsic characteristics of untrained 2D-Si, especially the quantum mechanical confinements (QMC), in order to design a future device.

In this work, we experimentally studied the large impact of the surface oxide layer on both E_G modulation and phonon confinement effects (PCE) of SQW. By etching process of the surface oxide layer of SQW, we demonstrated that E_G of SQW, evaluated by PL method, rapidly increases with decreasing the T_{OX}, which is attributable to the T_{OX} dependence of tensile strain in the SQW. On the other hand, QCE of SQW are not affected even by high temperature postannealing process after forming SQW.

II. Experimental Procedure for SQW

To study the impact of T_{OX} on QCE of SQW **(Fig.1)**, SQW with thin T_{OX} (1nm<T_{OX}≤12nm) was fabricated by wet-etching the surface oxide of initial SQW (i-SQW) with T_{OX} =120nm formed by dry oxidation of (100) bonded SOI substrate (T_S=55nm and buried oxide thickness T_{BOX}=145nm) at 1000°C (T_O) [4]. Tensile strain in SQW is applied by a thermal contraction mismatch between 2D-Si and surface oxide layers during a temperature drop from T_O to room temperature T_R (30°C), after forming the surface oxide layer which acts as a stressor layer for SQW. As a reference, strained SQW (s-SQW) was also fabricated by SSOI substrate with 0.7% tensile strain. T_{OX} and T_S were measured by UV/visual reflection method [4]. Minimum T_S and T_{OX} were 0.4 nm and 1.1 nm (natural oxide).

Next topic in this work is to study a thermal stability of QCE in SQW for future CMOS process. Thus, N_2 postannealing process at annealing temperature T_A for i-SQW was carried out in the range of 700°C≤T_A≤1100°C for 1-hour.

Using a 2D shear elastic stress simulator [10], 2D stress profile in i-SQW can be simulated in the condition of thermal contraction during a temperature drop T_O (1000°C) to T_R. According to an elastic energy E_E balance between each layer, E_E decrease with decreasing a layer thickness [11], and $E \propto T_S^{0.226}$ [9], the strain ε of 2D-Si rapidly increases with decreasing T_S **(Fig.2(a))**, which means that the impact of the surface-oxide layer on 2D-Si drastically increases with decreasing T_S. On the other hand, the stress P slightly decreases at T_S of 0.5nm, because of P=εE and E reduction [9]. In the case of SQW w/o surface oxide, P of 2D-Si slightly decreases **(Fig.2(b))**, because of no surface stressor oxide layer.

We analyzed the E_G properties of SQW evaluated by PL method with 2.33eV excitation laser, and stress/strain and PCE properties by a UV (325 nm) Raman spectroscopy [4]. Laser power P_L was 1mW to compress the P_L heating of Si [4], and the laser diameter is 1μm.

III. Surface Oxide Thickness Effects

(100) 2D-Si has a direct bandgap structure [2], and thus the peak PL energy E_{PH} is considered to be equal to the E_G of the 2D-Si [2], [4].

UV-Raman spectra show that an asymmetrical broadening W_L of SQW due to PCE [4] is almost independent of T_{OX}, and W_L≈120 cm^{-1} **(Fig.3(a))**. However, Raman peak downshift $\Delta\omega$ from 520 cm^{-1} of unstrained 3D-Si, decreases with decreasing T_{OX} **(Figs.3(a) and (b))**, which means that the tensile strain of SQW is partially relaxed by decreasing T_{OX}. Thus, assuming that $\Delta\omega$ is caused by the strain in the 2D-Si, experimental strain ε (%) decreases with decreasing T_{OX}, and can be well fitted by the following equation:

$$\varepsilon = 0.128\ln(1.39T_{OX}) \quad (1).$$

As a result, the ε value (~0.34%) is almost the same as simulated one at thicker T_{OX} (120nm), but is much lower than the simulation result of SQW w/o oxide layer **(Fig.3(b))**. Thus, this is the limitation of stress simulator for thinner T_{OX}.

On the other hand, PL spectra show strong dependence of T_{OX} **(Fig.4(a))**. E_G of the SQW increases with decreasing T_{OX} **(Fig.4(b))**, where $E_G \propto T_{OX}^{-0.021}$. As a result, E_G at T_{OX} =1.1nm is larger by 0.15eV than that at T_{OX} =120nm. The T_{OX} dependence of E_G suggests that E_G of SQW depends on the strain of 2D-Si. Actually, experimental PL spectra **(Fig.5(a))** show that s-SQW has about 50 meV lower E_G, compared to that of i-SQW, which is probably attributable to the strain induced subband splitting [12] even in 2D layers, as well as the subband modulation in unstrained ETSOI [13]. As a result, according to Figs. 3(a), 4, and 5(a), it is obvious that E_G of SQW rapidly increases with decreasing ε **(Fig.5(b))**, that is,

$$E_G = 1.65\varepsilon^{-0.058} \quad (2).$$

Eq. (2) shows the strain induced bandgap lowering (SIBL) effects. Thus, unstrained SQW w/o surface stressor oxide has larger E_G value.

Here, we summarize the E_G of SQW as a function of T_S **(Fig.6)**. E_G saturation of SQW at T_{OX} =120nm in T_S <0.8 nm is considered to be attributable to the SIBL of SQW. E_G of SQW at T_{OX} =1.1nm is larger than that of SQW at T_{OX} =120nm, but is still lower than theoretical results [14]. Physical mechanism for the discrepancy between this work and the theory is not understood at present, but is possibly due to the influence of the Si surface state on the E_G of SQW.

IV. Thermal Stability of 2D-Si

$\Delta\omega$ difference $\delta\Delta\omega$ is introduced by $\delta\Delta\omega \equiv \Delta\omega_A - \Delta\omega_B$, where $\Delta\omega_A$ and $\Delta\omega_B$ are Raman peak downshift of i-SQW after and before postanneling process, respectively. In spite of increasing T_A, $\delta\Delta\omega$ values keep constant **(Fig.7)**. Therefore, even at high T_A of lower than 1100°C, the strain of SQW is not relaxed by the slip at the interface between 2D-Si and oxide layer.

Furthermore, E_G of i-SQW evaluated by PL method is independent of T_A **(Fig.8)**. Therefore, the band structure of SQW is not affected by the postannealing process in T_A of lower than 1100°C, because of no T_A dependence of ε **(Fig.7)**.

VII. Conclusion

We experimentally studied the impact of the surface oxide stressor layer on QCE in Si quantum well structures. UV-Raman data show that tensile strain of SQW, applied by a thermal expansion mismatch between oxide and Si layers, decreases with decreasing the T_{OX}. As a result, PL results show that E_G of the SQW rapidly expands with decreasing T_{OX}, which is due to SIBL in SQW. However, SQW characteristics can keep thermally stable in spite of high temperature postannealing. Therefore, it is very important to consider the oxide stress effect on the SQW characteristics, in designing a future CMOS devices composed of 2D-Si structures.

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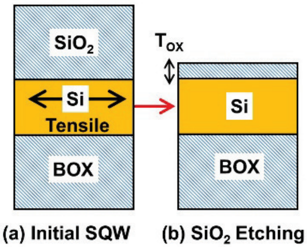
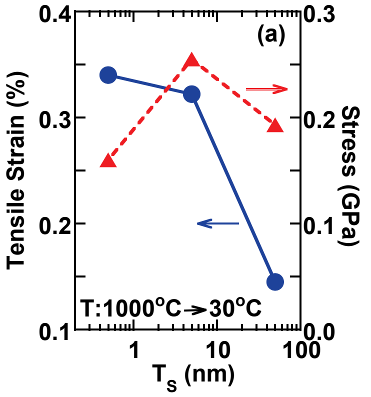


Fig.1 Schematic cross section of (a) initial SQW with surface oxide thickness T_{OX} of 120nm, and (b) SQW with various T_{OX} after etching a surface oxide of i-SQW. Tensile strain of SQW by the thermal contraction mismatch between surface oxide and 2D-Si, during a temperature drop from T_O to T_R, is considered to decrease with decreasing T_{OX}.



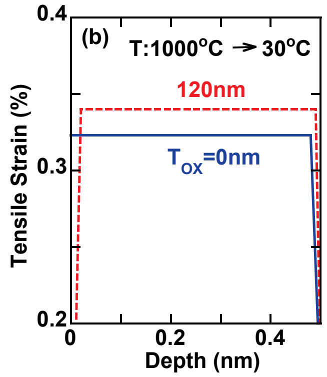


Fig.2 (a) Simulated tensile stress/strain in SQW with T_{OX}=120nm vs. T_S, and (b) tensile strain distribution from the Si surface in 0.5-nm SQW with T_{OX}=0nm (solid line) and 120nm (dashed line) with T_{OX}=120nm, in the condition of thermal contraction of temperature drop ΔT=970°C, where T_{BOX}=145nm. In this work, α_S and α_{OX} are 2.6×10^{-6} and 5×10^{-7}/°C [8], respectively, and $E \propto T_S^{0.226}$ [9].

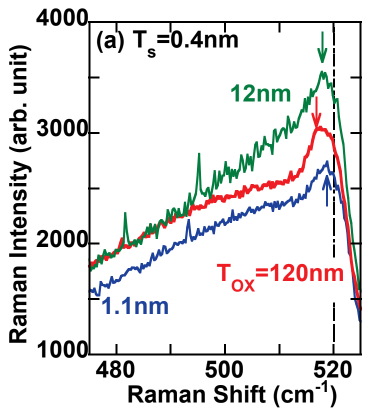


Fig.3 (a)

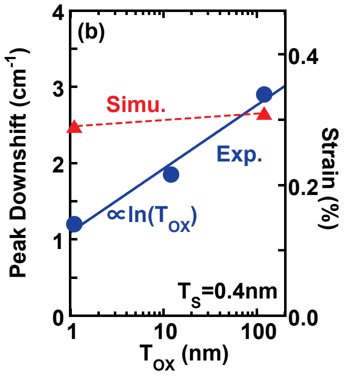
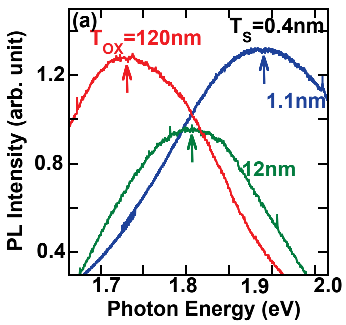


Fig.3 T_{OX} dependence of (a) UV-Raman spectra and (b) peak downshift/strain (circles) of SQW, where T_S=0.4nm. Arrows in (a) show the Raman peaks. Triangles in (b) shows simulation strain values ε, whose strain at T_{OX}=120nm is almost the same as the experimental strain. Fitting curve (solid line) in (b) shows that $\Delta\omega = 1.09\ln(1.39T_{OX})$ and $\varepsilon = 0.128\ln(1.39T_{OX})$, where the correlation coefficient is 0.98.



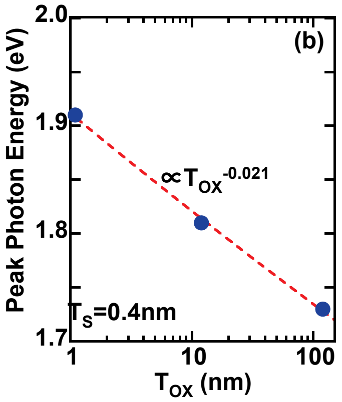


Fig.4 (a) PL spectra of SQW with various T_{OX} and (b) E_{PH} vs. T_{OX} in SQW (circle), where T_S=0.4nm. E_{PH} rapidly increases with decreasing T_{OX}. Dashed line shows the fitting curve of $E_{PH} \propto T_{OX}^{-0.021}$ with the correlation coefficient of 0.999.

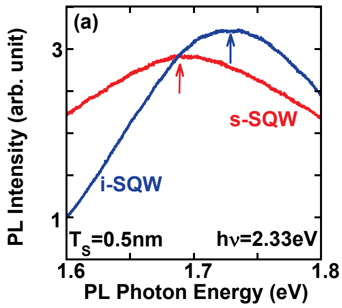


Fig.5 (a)

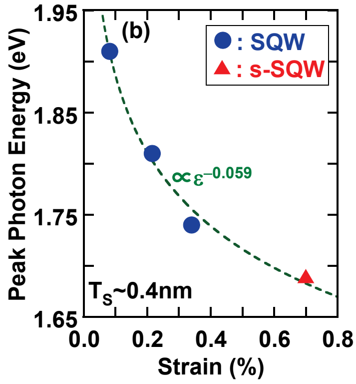


Fig.5 (a) PL spectra of s-SQW with 0.7% tensile strain and i-SQW, where T_S≈0.5nm and T_{OX}≈120nm. (b) E_G vs. experimental strain values obtained by Fig.3(b) (circles) and 5(a) (triangle). Dashed line shows the fitting curve of $E_G \propto \varepsilon^{-0.059}$ with the correlation coefficient of 0.99.

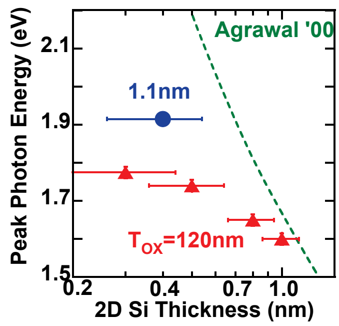


Fig.6 E_G vs. T_S in SQW with T_{OX}=1.1nm (circle) and i-SQW with T_{OX}=120nm (triangles). The dashed line shows theoretical results [14]. Error bars show the T_S variation in a 10^4 μm^2 area [4].

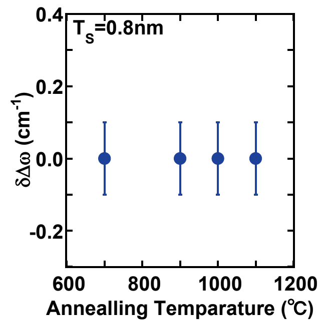


Fig.7 UV-Raman peak downshift difference of i-SQW before and after postannealing process, as a function of T_A, where T_S=0.8nm and T_{OX}=120nm. Error bars show the Raman resolution in this study.

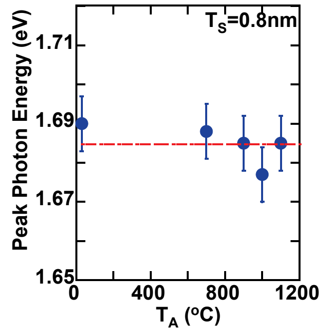


Fig.8 E_G vs. T_A in i-SQW, where T_S=0.8nm and T_{OX}=120nm. Error bars show the PL resolution in this study.