Anisotropic Phonon-Confinement-Effects/Band-Structure-Modulation of Two-Dimensional Si Lavers Fabricated on Silicon-on-Quartz Substrates

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Abstract

We have experimentally studied anisotropic phonon confinement effects and E_G modulation of a two dimensional (2D) Si on silicon-on-quartz (SOQ) substrates, using polarization Raman and PL methods. For the first time, we demonstrated that PCE relaxes the Raman selection rule of 2D-Si with less than 1nm, especially at the polarization laser direction of about [001]. However, the E_G values caused by the band modulation are isotropic in the 2D-Si. On the other hand, absorption coefficient of the 2D-Si rapidly increases with decreasing T_S (<several nm), which is considered to be attributable to the band structure modulation of 2D-Si.

I. Introduction

2D-Si structures are very suitable for extremely-thin SOI (ETSOIs) and FinFET CMOS [1], as well as Si photonic devices [2]. To improve short channel effects (SCE) of CMOS and photoluminescence (PL) intensity of Si photonic devices, the 2D-Si thickness T_S is necessary to continue decreasing. Low-D Si nanostructures (Si nanowires (1D) and nanocrystals (0D)) [3] show strong quantum mechanical confinements (QMC), including phonon confinement effects (PCE) caused by the Heisenberg uncertainty principle of phonon wave vector Δq in a finite Si size. The PCE induces the carrier mobility reduction due to the enlarged phonon scattering of carriers [3]. Recently, we have experimentally studied the asymmetrical broadening of Raman intensity due to PCE and bandgap E_G modulation (BM) in (100)/(110) 2D-Si layers on buried oxide (BOX) with $T_S \approx a$ (Si lattice constant) [4-5]. However, other optical properties of 2D-Si, such as the relaxation effect of the Raman selection rule caused by the PCE [6] and photon absorption properties modulation, have not been studied in detail, yet, because the optical intensities from the Si substrate under the BOX are relatively large, compared with those of the surface thin 2D-Si.

In this work, we have experimentally made clear anisotropic PCE and BM of 2D-Si layers on (100)-surface SOQ wafer without Si substrate under the BOX, using polarization Raman and photoluminescence (PL) methods. We demonstrated that the Raman selection rule of the PCE is anisotropically relaxed, but the PL peak energy E_{PH} is isotropic. II. Experimental for 2D-Si Layers on SOQ

2D-Si was fabricated by a thermal oxidation (Dry-O2) process of (100)SOQ at high temperature (1000°C). Thus, we can directly measure the optical properties of 2D-Si in detail, because of no Si layer beneath the BOX. The T_S of 2D-Si layers is mainly evaluated by UV/visual reflection spectrum, which is also verified by HRTEM [4]. We formed 0.5nm 2D-Si on SOQ (Fig.1).

We measured the anisotropic PCE and BM by a polarization 442nm-Raman spectroscopy and PL of an excitation laser photon energy hv (*h* is Planck constant and *v* is photon frequency) of 2.33eV (532nm) at room temperature, respectively, where the laser power is 1mW to avoid the laser power induced heating effects of the 2D-Si [5], and the laser diameter is 1 μ m. An absorption coefficient of 2D-Si was evaluated by the UV/visual reflection *R* and transmission T spectra.

III. Anisotropic Phonon Confinement Effects

Using Raman scattering vector (\vec{k}_s) geometry of an incident laser beam vector (\vec{k}_l) onto (100) 2D-Si, where the polarization laser and Raman vectors are \vec{E}_I and \vec{E}_S , respectively (Fig.2), the Raman intensity I_R can be determined by the Raman selection rule, that is, $I_R \propto \sum_I |\vec{E_I} R_I \vec{E_S}|^2$, where R_J is Raman tensor of phonon J for 3D-Si [7]. In the case of (100) 3D-Si, $I_R \propto \cos^2(2\phi + \theta)$ (1) [7].

We have experimentally confirmed that the asymmetrical broadening W_L of SOQ in 442nm-Raman spectra rapidly increases in $N_L < 30$, and has the same Si layer number $N_L (\equiv T_S/d+1)$ as W_L of 325nm-Raman spectra of both SOQ and SOI [5] (Fig.3), where W_L

is full-width-tenth-maximum of I_R at lower wave number region from 520cm⁻¹ caused by PCE [5] and d (0.136nm) is the minimum distance between Si atoms at (100) 2D-Si [5]. Thus, we use 442nm Raman spectroscopy data for evaluating the PCE.

Figs.4(a) and 4(b) show polarization Raman spectra of 2D-Si with T_s of 1nm at the polarization laser direction of [011] ($\phi=0^\circ$) and [001] (ϕ =45°), respectively. At ϕ =0°, I_R of both the 520cm peak and asymmetrical broadening region disappears at θ =90° (Fig.4(a)), which is obeyed by the Raman selection rule (Eq.(1)). However, at $\phi=45^\circ$, I_R at asymmetrical broadening region is not polarized, that is, I_R at $\theta=0^\circ$ equals to I_R at $\theta=90^\circ$ (Fig.4(b)), which is the relaxation effects of the Raman selection rule due to PCE [6]. In addition, I_R of 520cm⁻¹ peak at θ =90° is reduced, but is not zero.

In this study, we experimentally demonstrated the Raman selection rule at the first-order Raman scattering of 520cm⁻¹, since the experimental ϕ dependence of the I_R of both 56-nm SOQ (Fig.5(a)) and 1-nm 2D-Si (Fig.5(b)) can be explained by the theoretical $\cos^2(2\phi + \theta)$ dependence. On the other hand, I_R of 1-nm 2D-Si at asymmetrical broadening region of 480cm⁻¹ deviates from the $\cos^2(2\phi + \theta)$ dependence especially at $\phi \approx 45^\circ$ ([001]) (Fig.5(c)). This ϕ uncertainty $\Delta \phi$ becomes about 15° (Fig.5(c)). Thus, we have experimentally verified that PCE relax the Raman selection rule in the 2D-Si, which is due to the Δa .

IV. Isotropic Bandgap Modulation

Using the polarization PL method, we have studied anisotropic E_G characteristics of 2D-Si evaluated by the peak PL photon energy

 E_{PH}^{-} . We experimentally confirmed that the E_{PH} of 1.66eV of 0.8nm 2D-Si at the [011] direction is almost equal to that (1.67eV) at the [001] direction (Figs.6). In addition, the E_{PH} of SOQ is the same value as that of 0.8nm SOI [5]. Consequently, the E_G values due to the band structures modulation in the 2D-Si are isotropic.

V. Absorption Coefficient Increase

In this study, we can directly measure the absorption coefficient α of the 2D-Si of SOQ as a function of T_S , and thus, we discuss the band structure modulation of 2D-Si.

Photon flux I_F absorbed in the 2D-Si with T_S is given by $I_F = (1 - R)I_0(1 - e^{-\alpha T_S})$, where I_0 is the incident photon flux at the Si surface. Thus, $1 - R - T = (1 - R)(1 - e^{-\alpha T_S})$, resulting in $\alpha = \ln((1-R)/T)/T_s$ (2). Therefore, α of the 2D-Si can be obtained by measuring both the reflection *R* and transmission *T* spectra of SOQ (Fig.7).

The α of the 56nm SOQ is completely equal to that of bulk Si reference [8] (Fig.7(a)), and thus we verified that this method (Eq.(2)) to evaluate the α is valid. With decreasing T_s the α increases in the whole range of the photon energy (Fig.7(a)). However, we cannot detect the α edge, because of higher noise level of R and T at lower hv. At hv=2eV, the α rapidly increases, and the α in $T_{S} \leq 1$ nm is one order of magnitude larger than that in T_s >4nm (Fig.7(b)), which causes the remarkable increase of the PL intensity of 2D-Si [5]. However, the α increasing rate $d\alpha/dT_s$ slightly decreases with increasing $h\nu$ (Fig.7(b)). The rapid increase of α (Figs.7) [8] suggests that the band structure of 2D-Si modulates to direct bandgap transmission from indirect one of 3D-Si.

VI. Conclusion

We have experimentally made clear anisotropic phonon confinement effects and E_G modulation of the 2D-Si on SOQ, using polarization Raman and PL methods. Moreover, absorption coefficient of the 2D-Si rapidly increases with decreasing T_S (<several nm), which is attributable to the band structure modulation of 2D-Si. Consequently, it is necessary to reconstruct the device design for CMOS composed of the 2D-Si structures, considering the anisotropic quantum mechanical confinements in the 2D-Si.

Acknowledgement: This work was partially supported by KAKENHI (24560422). 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, JJAP 51, 02BC03, 2012. [5] T. Mizuno, JJAP 52, 04CC13, 2013. [6] S. Piscanec, Phys. Rev., B68, 241312, 2003. [7] K. Mizoguchi, JAP, 65, 2585, 1989. [8] S. M. Sze, Physics of Semiconductor Devices (Wiley), 2007.



Fig.1 UV/visual reflectivity spectrum (solid line) of 0.5nm 2D-SOQ. The dashed line is the fitting curve and shows that $T_s \approx 0.5$ nm.



Fig.2 Raman scattering geometry on (100) 2D-Si surface. The [100] axis shows the surface orientation of the 2D-Si plane. \vec{k}_I and \vec{E}_I with the angle ϕ between the [011] axis are the incident and polarization laser vectors onto the (100) 2D-Si, respectively. \vec{k}_S and \vec{E}_S with the angle θ between \vec{E}_I are the scattered and polarization Raman photon vectors, respectively.



Fig.3 N_L dependence of W_L of SOQ (squares) and SOI (triangles) evaluated by 325nm-laser Raman. Circles show the 442nm-laser Raman data of SOQ.





Fig.4 Polarization 442nm-Raman spectra of (a) $\phi=0^{\circ}$ ($\vec{E}_{I} = [011]$) and (b) $\phi=45^{\circ}$ ($\vec{E}_{I} = [001]$), where $T_{5}\approx$ 1nm. The solid and dashed lines show the data of $\theta=0^{\circ}$ and 90° , respectively. DT (solid and dotted line) shows the detection limit for the polarization Raman spectroscopy in this study.



Fig.5 ϕ dependence of polarization 442nm-Raman region of promalized by the peak intensity for (a) 520 cm⁻¹ peak at T_s =56nm, (b) 520 cm⁻¹ peak at T_s =1nm, (c) 480 cm⁻¹ of PCE region at T_s =1nm. Circles and squares show the data of $\theta=0^{\circ}$ and 90°, respectively. The dashed (θ =0°) and dotted (θ =90°) lines show the theoretical results of $\cos^2(2\phi + \theta)$ dependence [7].





Fig.6 Polarization PL spectra of (a) $\phi=0^{\circ}$ ($\vec{E}_I = [011]$) and (b) $\phi=45^{\circ}$ ($\vec{E}_I = [001]$), where $T_S \approx 0.8$ nm and excitation photon energy hv=2.33 eV. The arrows show the peak PL photon energy E_{PH}



Fig.7 (a) Absorption coefficient α spectra of SOQ with various T_s and (b) T_s dependence of α in various photon energies. The dotted line in Fig.(a) shows experimental α spectrum of 3D-Si [8].