Anisotropic Phonon-Confinement-Effects/Band-Structure-Modulation of Two-Dimensional Si Layers Fabricated on Silicon-on-Quartz Substrates
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Abstract
We have experimentally studied anisotropic phonon confinement effects and \( E_c \) modulation of a two dimensional (2D) Si on silicon-on-quartz (SOQ) substrates, using polarization Raman and PL methods. For the first time, we demonstrate \( E_c \) 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 \( E_c \) 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 \( T_S \) (seven 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 (ETSOs) and FinfET CMOS [1], as well as Si photonic devices [2]. To improve short channel effects (SCE) of CMOS and 

\( \text{III. Anisotropic Phonon Confinement Effects} \)
Using Raman scattering vector \( \vec{k}_R \) geometry of an incident laser beam vector \( \vec{k}_L \) onto (100) 2D-Si, where the polarization laser and Raman vectors are \( \vec{E}_L \) and \( \vec{E}_S \), respectively (Fig.2), the Raman intensity \( I_R \) can be determined by the Raman selection rule, that is, 

\[ I_R \propto \left| \sum E_R E_S \right|^2, \]

where \( E_R \) is Raman tensor of phonon \( J \) for 3D-Si [7]. In the case of (100) 3D-Si, 

\[ I_R \propto \cos^2(2\theta + \theta) \]  

(1) [7].

We have experimentally confirmed that the asymmetrical broadening \( W_T \) of SOQ in 442nm-Raman spectra rapidly increases in \( \lambda / 30 \), and has the same Si layer number \( N_L = (\text{with } 32\text{nm-Raman spectra of both SOQ and SOI}[5] \text{Fig.3}), \text{where } W_T \text{ is full-width-half-maximum of } I_P \text{ at lower wave number region from } 520cm^{-1} \text{ caused by } E_P \text{ [5] and } \theta (0.136nm) \text{ is the minimum distance between Si atoms at } (100) 2D-Si [5]. \text{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 \text{ of 1nm at the polarization laser direction of } [011] (\phi = 0^\circ) \text{ and } [001] (\phi = 45^\circ), \text{respectively. At } \phi = 0^\circ, I_P \text{ of both the } 520cm^{-1} \text{ peak and asymmetrical broadening region disappears at } \theta = 90^\circ \text{ (Fig.4(a)), which is obeyed by the Raman selection rule (Eq.(1)). However, at } \phi = 45^\circ, I_P \text{ at asymmetrical broadening region is not polarized, that is, } I_P \text{ at } \theta = 0^\circ \text{ equals to } I_P \text{ at } \theta = 90^\circ \text{ (Fig.4(b)), which is the relaxation effects of the Raman selection rule due to PCE [6] in addition, } I_P \text{ of } 520cm^{-1} \text{ peak at } \theta = 90^\circ \text{ 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}, \text{since the experimental } \phi \text{ dependence of the } I_P \text{ 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\theta + \theta) \text{ dependence. On the other hand, } I_P \text{ of 1-nm 2D-Si at asymmetrical broadening region of } 480cm^{-1} \text{ deviates from the } \cos^2(2\theta + \theta) \text{ dependence especially at } \phi = 45^\circ \text{ (001) (Fig.5(e)). This } \phi \text{ uncertainty } \Delta \phi \text{ becomes about } 15^\circ \text{ (Fig.5(c)). Thus, we have experimentally verified that PCE relax the Raman selection rule in the 2D-Si, which is due to the } \Delta \phi. \text{IV. Isotropic Bandgap Modulation} \text{Using the polarization PL method, we have studied anisotropic } E_G \text{ characteristics of } 2D-Si \text{ evaluated by the peak PL photon energy } E_P. \text{We experimentally verified that the } E_G \text{ of } 2.33eV \text{ at room temperature, respectively, where the laser photon frequency) of } 532nm \text{ at room temperature, respectively, where the laser power is } 1mW \text{ to avoid the laser power induced heating effects of the 2D-Si [5], and the laser diameter is } 1\mu m. \text{An absorption coefficient of } 2D-Si \text{ was evaluated by the UV/visible 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 of a polarization 442nm-Raman spectroscopy and PL of an exciton laser photon energy } h \nu \text{ (h is Planck constant and } \nu \text{ is photon frequency) of } 2.33eV \text{ (532nm) at room temperature, respectively, where the laser power is } 1mW \text{ to avoid the laser power induced heating effects of the 2D-Si [5], and the laser diameter is } 1\mu m. \text{An absorption coefficient of } 2D-Si \text{ was evaluated by the UV/visible reflection R and transmission T spectra.} \]

III. Anisotropic Phonon Confinement Effects
Using Raman scattering vector \( \vec{k}_R \) geometry of an incident laser beam vector \( \vec{k}_L \) onto (100) 2D-Si, where the polarization laser and Raman vectors are \( \vec{E}_L \) and \( \vec{E}_S \), respectively (Fig.2), the Raman intensity \( I_R \) can be determined by the Raman selection rule, that is, 

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We have experimentally confirmed that the asymmetrical broadening \( W_T \) of SOQ in 442nm-Raman spectra rapidly increases in \( \lambda / 30 \), and has the same Si layer number \( N_L \) as \( W_T \) of 32nm-Raman spectra of both SOQ and SOI [5] (Fig.3), where \( W_T \) is full-width-half-maximum of \( I_P \) at lower wave number region from 520cm\(^{-1}\) caused by \( E_P \) [5] and \( \theta (0.136nm) \) 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 \([001]\) (\(\phi = 45^\circ\)), respectively. At \(\phi = 0^\circ\), \( I_P \) of both the 520cm\(^{-1}\) peak and asymmetrical broadening region disappears at \(\theta = 90^\circ\) (Fig.4(a)), which is obeyed by the Raman selection rule (Eq.(1)). However, at \(\phi = 45^\circ\), \( I_P \) at asymmetrical broadening region is not polarized, that is, \( I_P \) at \(\theta = 0^\circ\) equals to \( I_P \) at \(\theta = 90^\circ\) (Fig.4(b)), which is the relaxation effects of the Raman selection rule due to PCE [6]. In addition, \( I_P \) of 520cm\(^{-1}\) peak at \(\theta = 90^\circ\) 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 \(\phi\) dependence of the \( I_P \) of both 56-nm SOQ (Fig.5(a)) and 1-nm 2D-Si (Fig.5(b)) can be explained by the theoretical \(\cos^2(2\theta + \theta)\) dependence. On the other hand, \( I_P \) of 1-nm 2D-Si at asymmetrical broadening region of 480cm\(^{-1}\) deviates from the \(\cos^2(2\theta + \theta)\) dependence especially at \(\phi = 45^\circ\) (001) (Fig.5(e)). This \(\phi\) uncertainty \(\Delta \phi\) becomes about \(15^\circ\) (Fig.5(c)). Thus, we have experimentally verified that PCE relax the Raman selection rule in the 2D-Si, which is due to the \(\Delta \phi\).

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

Fig.2 Raman scattering geometry on (100) 2D-Si surface. The [100] axis shows the surface orientation of the 2D-Si plane. $E_i$ and $E_f$ with the angle $\phi$ between the [011] axis are the incident and polarization laser vectors onto the (100) 2D-Si, respectively. $E_i$ and $E_f$ with the angle $\theta$ between $E_f$ are the scattered and polarization Raman photon vectors, respectively.

Fig.3 Number of Si Atom Layers dependence of $W_e$ 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) $\phi=0^\circ$ ($E_i=011$) and (b) $\phi=45^\circ$ ($E_i=001$), where $T_S=1nm$. The solid and dashed lines show the data of $\phi=0^\circ$ and $90^\circ$, respectively. DT (solid and dotted line) shows the detection limit for the polarization Raman spectroscopy in this study.

Fig.6 Polarization PL spectra of (a) $\phi=0^\circ$ ($E_i=011$) and (b) $\phi=45^\circ$ ($E_i=001$), where $T_P=0.8nm$ and excitation photon energy $h\nu=2.33eV$. The arrows show the peak PL photon energy $E_{ph}$.

Fig.5 $\phi$ dependence of polarization 442nm-Raman intensity normalized by the peak intensity for (a) 520cm$^{-1}$ peak at $T_s=56nm$, (b) 520cm$^{-1}$ peak at $T_s=1nm$, (c) 480cm$^{-1}$ of PCE region at $T_s=1nm$. Circles and squares show the data of $\phi=0^\circ$ and $90^\circ$, respectively. The dashed ($\phi=0^\circ$) and dotted ($\phi=45^\circ$) lines show the theoretical results of $\cos^2(2\phi + \theta)$ dependence [7].

Fig.7 Absorption coefficient $\alpha$ spectra of SOQ with various $T_s$ and $E_{ph}$ dependence of $\alpha$ in various photon energies. The dotted line in Fig.(a) shows experimental $\alpha$ spectrum of 3D-Si [8].