\[ \Delta E_G = 15.7 \ln(N/3.32 \times 10^7) \]  

(1)

Thus, the coefficient of \( N \) in Eq. (1) is larger by about two orders of magnitude that of 3D-Si [6]. However, \( \Delta E_G \) difference between p' 2D-Si and 3D-Si is very small (Fig.7). Consequently, the reduced \( \Delta E_G \) is the characteristic of doped 2D-Si, and depends on the dopant type.

IV. Impurity Band Modulation (IBM) of Doped 2D-Si

To explain the \( \Delta E_G \) difference between 2D- and 3D-Si (Fig.7), we consider that there are two possible mechanisms. One is the donor deactivation effects in the 2D-Si, and the other is IBM. Using the former model, the donor activation rate in the 2D-Si should be reduced by about two orders of magnitude, compared to that of 3D-Si (Fig.7). However, the possibility of the above larger deactivation is very low, because even in 1D-Si, the donor activation rate is reduced by only one order of magnitude [8]. Thus, we introduce the IBM model in this study (Fig.8).


N+ / P+ Single Doping Effects on Impurity Band Structure Modification in Two Dimensional Si Layers

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Abstract

We experimentally studied n' p' single dopant atom effects on band structure modulation in 2D-Si layers in a wide range of dopant density \( N \), using photoluminescence (PL) method. Bandgap \( E_G \) of both n' p' 2D-Si strongly depends on the \( N \), and decreases with increasing \( N \), which is attributable to \( E_G \) narrowing effects of both n' and p' 2D-Si layers. The reduced \( \Delta E_G \) is much smaller than that of 3D-Si and depends on the dopant type.

We introduce a simple model for the small \( \Delta E_G \) considering the impurity band structure modulation in a heavily doped 2D-Si. Moreover, small PL polarization of doped 2D-Si is also discussed.

In two dimensional (2D) Si layers, which are key structures for realizing extremely-thin SOIs (ETSOIs) and FinFET CMOS [1], as well as Si photonic devices [2], we experimentally demonstrated phonon confinement effects (PCE) caused by the Heisenberg’s uncertainty principle, and the phonon wave vector and bandgap \( (E_G) \) expanding due to electron confinement effects [3]-[5]. Moreover, in the case of an n' 2D-Si in less than \( 4 \times 10^{10} \text{cm}^{-2} \), PL method show that \( \Delta E_G \) is reduced [5], compared to that of 3D-Si [6]. The \( \Delta E_G \) of 3D-Si is attributable to the impurity band of donors including the band tailing [7]. Moreover, donor level modulation in an 1D-Si is reported [8]. To design a pn junction of CMOS composed of 2D-Si in detail, it is strongly required to clarify both the reduced \( \Delta E_G \) effects in detail and the physical mechanism in both n' and p' 2D-Si in a wide range of dopant density.

In this work, we experimentally studied the n' p' single dopant atom effects on the band structures in doped 2D-Si layers fabricated by ion implantation, using PL method. We confirmed that \( E_G \) strongly depends on an impurity dopant density \( N \), and decreases with increasing \( N \). However, \( \Delta E_G \) in the doped 2D-Si is is much smaller than that in 3D-Si. The reduced \( \Delta E_G \) in doped 2D-Si is possibly attributable to the impurity band modulation (IBM) effects in doped 2D-Si. Next, we show small PL polarization in a doped 2D-Si, which is possibly caused by the disturbed crystal direction due to heavy impurity dopant.

II. Experimental for Doped 2D-Si Layers

To control 2D-Si thickness \( T_S \) very well, n' and p' 2D-Si layers were fabricated by two-step (low-temperature (T) after high-T oxidation) thermal oxidation induced thinning of (100) bonded SOI substrates (Figs.1 and 2). In addition, B' for acceptor ions were implanted in different process steps (Figs.1 and 2), considering the P' and B' segregation coefficients \( m \) at the Si/SiO\(_2\) interface, during the oxidation of SOI substrates, are about 10 and 0.1, respectively [5], [9].

HRTM observation shows very uniformity and good crystal quality of n' 2D-Si layer even at higher N condition (Fig.3), which is the same image as HRTM result of intrinsic 2D-Si [3].

SIMS results for boron profile in a doped 2D-Si show that average of experimental boron density \( N_B \) is almost the same as the 2D simulation results [10] (Fig.4), although the SIMS profile at the oxide/Si interfaces is inaccurate, because of the SIMS detection limit. Thus, in this study, N of 2D-Si in various ion implantation conditions can be obtained by the simulation results [10].

We analyzed the \( E_G \) properties of n' p' 2D-Si evaluated by PL method with 2.33eV excitation laser at room temperature [4]. Laser power \( P_L \) was 1mW to compress the \( P_T \) heating of Si [4], and the laser diameter is \( 1 \mu m \).

III. Dopant Density Dependence of \( \Delta E_G \)

N dependence of PL spectra shows that PL intensity \( I_{PL} \) and \( E_G \) in both n' p' 2D-Si decreases with increasing \( N \) (Figs.5 and 6), where \( E_G \approx \frac{N}{0.009} \) in both n' p' 2D-Si (Fig.6). However, the N dependence in p' 2D-Si is much different from that of n' 2D-Si (Fig.6).

The reduced \( E_G \) in both n' p' 2D-Si is attributable to the \( \Delta E_G \) caused by the impurity band in a degenerate Si [7], [8]. Here, \( \Delta E_G = E_G - E_G\)~0D, where \( E_G\) and \( E_G\) are \( E_G \) of intrinsic and doped 2D-Si, respectively (Figs.6-8(a)). \( \Delta E_G \) of n' 2D-Si is much smaller than that of 3D-Si (\( \Delta E_G = 18.7 \ln(N/7 \times 10^7) \) [6], and the \( \Delta E_G \) of n' 2D-Si can be well fitted by the following equation (Fig.7):
Fig. 1 Schematic two-step oxidation fabrication process for 2D-n+ layers. (a) After P+ implantation into (100)SOI, (b) Si was thinned by high temperature oxidation (1000°C). (c) Additional low-T oxidation (900°C) after (b) was carried out to form nm-region thick Si layer.

Fig. 2 Schematic two-step oxidation fabrication for 2D-p+ layers. (a) After high-T oxidation process (1000°C), (b) B+ was implanted into thinned (100)SOI. (c) Additional low-T oxidation (900°C) after (b) was carried out to form nm-region thick Si layer.

Fig. 3 HRTEM observation of cross section of 2D-n+ layer with \( N_B = 4 \times 10^{19} \text{cm}^{-3} \). (a) Very uniform 2D-n+ layer, and (b) good Si lattice image and \( T_S = 0.5 \text{nm} \).

Fig. 4 SIMS (solid line) and simulation distribution (dotted line) for boron atoms, where boron dose is \( 1 \times 10^{19} \text{cm}^{-2} \) and \( T_S = 4 \text{nm} \). Minimum \( T_S \) for SIMS detection limit is about several nm. Dashed line shows the experimental average of boron density (\( 1.8 \times 10^{19} \text{cm}^{-2} \)) in Si layer which is obtained by the SIMS data, and is almost the same level as the simulation result (\( 1.2 \times 10^{19} \text{cm}^{-2} \)) in Si.

Fig. 5 Dopant density dependence of PL spectra of (a) n+ and (b) p+ 2D-Si, where \( T_S = 0.5 \text{nm} \). Dotted and dashed line in (b) shows the E\(_{\text{IN}}\) of i-Si.

Fig. 6 \( E_{\text{PH}} \) vs. simulated impurity density of n+ (circles) and p+ 2D-Si (triangles), where \( T_S = 0.5 \text{nm} \). Dotted and dashed line shows the fitting curve of \( E_{\text{IN}} = N^{-0.009} \), where the correlation coefficient is 0.98.

Fig. 7 Bandgap narrowing vs. simulated impurity density of n+ (circles) and p+ 2D-Si (triangles), where \( T_S = 0.5 \text{nm} \). Solid line shows empirically formula of 3D-Si \([6]\). Dashed line shows the fitting curve of \( \delta E_{\text{IN}} = 15.7 \ln(N_B/3.32 \times 10^{19}) \) in n+ 2D-Si with the correlation coefficient of 0.98. \( \delta E_{\text{IN}} \) is \( E_{\text{IN}} \) modulation in n+ 2D-Si.

Fig. 8 Schematic density of states functions (\( E \) vs. DOS) for (a) n+ 3D-Si \([7]\) and (b) n+ 2D-Si with expanded \( E_{\text{IN}} \). Dashed and solid lines show the conduction and impurity bands, respectively. Dotted line in (b) shows the impurity band of 3D-Si. \( \delta E_{\text{IN}}, \delta E_{\text{C}}, \delta E_{\text{E}} \) are \( E_{\text{IN}} \) narrowing, \( E_{\text{C}} \) band width and \( E_{\text{E}} \) modulation, respectively.

Fig. 9 Impurity band structure modulation of n+ (circles) and p+ 2D-Si (triangles). \( \delta E_{\text{IN}} \) as a function of simulated dopant density, where \( T_S = 0.5 \text{nm} \). Both \( \delta E_{\text{IN}} \) and \( \delta E_{\text{CB}} \) are independent of dopant density, but \( \delta E_{\text{CB}} \) is much larger than \( \delta E_{\text{IN}} \).

Fig. 10 Polarization PL spectra of 2D-n+ layer in various \( \theta \) where \( N_B = 4 \times 10^{19} \text{cm}^{-2} \) and \( T_S = 0.5 \text{nm} \). \( E_{\text{IN}} \) at fixed [110] direction and \( E_{\text{IN}} \) in the inset show polarization laser and PL vectors, respectively, and \( \theta \) is the angle between \( E_{\text{IN}} \) and \( E_{\text{PL}} \).

Fig. 11 PL polarization degree of n+ (solid lines), p+ (dashed line), and intrinsic 2D-Si (dotted line) at \( E_{\text{IN}} = 110 \) as a function of \( \theta \), where \( T_S = 0.5 \text{nm} \).

Fig. 12 0 dependence of \( E_{\text{IN}} \) at \( \theta = 0^\circ \) (circles) and \( 90^\circ \) (triangles), where \( N_B = 2 \times 10^{19} \text{cm}^{-2} \) and \( T_S = 0.5 \text{nm} \). Inset shows the polarization laser angle \( \theta \) between [110] direction and \( E_{\text{IN}} \).