

Photoluminescence from Silicon Quantum Well Formed on SIMOX Substrate

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We have observed strong photoluminescence (PL) from a well defined two-dimensional (2D) Si structure formed on a SIMOX wafer, where the thin (< 5 nm) single crystalline silicon film is sandwiched between SiO₂ layers. It is found that the PL intensity has a sharp maximum at a Si thickness of about 2 nm, whereas the peak photon energy of the PL spectra (1.65 eV) is almost independent of the Si thickness. These results can be interpreted with a three-region model in which electron-hole pairs are excited in the Si well and luminescence occurs at the upper and lower Si/SiO₂ interfaces. Furthermore, temperature dependence of PL intensity in the present 2D system is found to be different from previously reported dependence in 0D or 1D structures.

1. INTRODUCTION

A great deal of attention has been concentrated on the mechanism of bright visible photoluminescence (PL) from porous Si^{1,2} because quantum confinement effects of the low dimensional Si structure might play a substantial role. In this system, however, it has been relatively difficult to precisely control the structure configuration and size. Therefore, little information is available about quantitative comparison between PL spectra and structure. Recently, similar PL was observed from nano-scale Si pillars (1D)³ formed by electron beam lithography and reactive ion etching and Si nanometer-sized spheres (0D)⁴ formed by laser breakdown of SiH₄ gas. Up to now, only 1D or 0D confinement has been studied for the PL from Si: more fundamental 2D systems have not been reported yet. We report, for the first time, strong PL from a SiO₂/Si/SiO₂ sandwiched two-dimensional (2D) Si structure. In this structure, the size is defined by the thickness alone. This enables us to analyze the size effect on PL within an acceptable range of experimental error.

2. EXPERIMENTAL

Figure 1 shows the sample structure used in the PL experiments. We started with a (100) SIMOX (Separation by Implanted Oxygen) wafer. The initial 140-nm superficial Si thickness was reduced to 5 nm or less by thermal oxidation. The 2D-Si is sandwiched between 30-nm-thick surface SiO₂ and 400-nm-thick

buried SiO₂ layers, as shown in Fig. 1. These thicknesses were measured by spectroscopic ellipsometry. Good crystalline quality in the Si layers, without a disordered transition layer near the Si/SiO₂ interfaces, was confirmed by cross-sectional TEM (transmission electron microscopy).

PL spectra were measured at 10 K by using a 488-nm (2.54 eV) excitation wavelength in an Ar⁺ laser. The typical laser power was 5 mW with a spot diameter of about 100 μm.

3. RESULTS AND DISCUSSIONS

Figure 2 shows the PL spectra for 2D-Si layers with various thicknesses. The PL intensity has a maximum at 2 nm and any no PL peak is observed when the Si layer is thicker than 5 nm. The peak photon energies of these spectra are plotted in Fig. 3 as

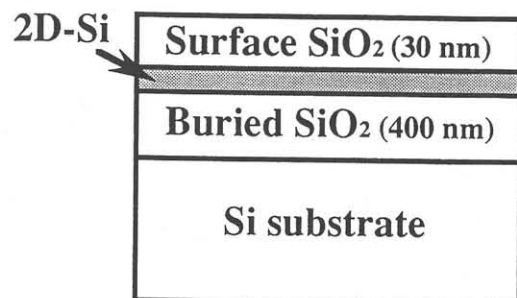


Fig. 1 Schematic cross-sectional view of the sample.

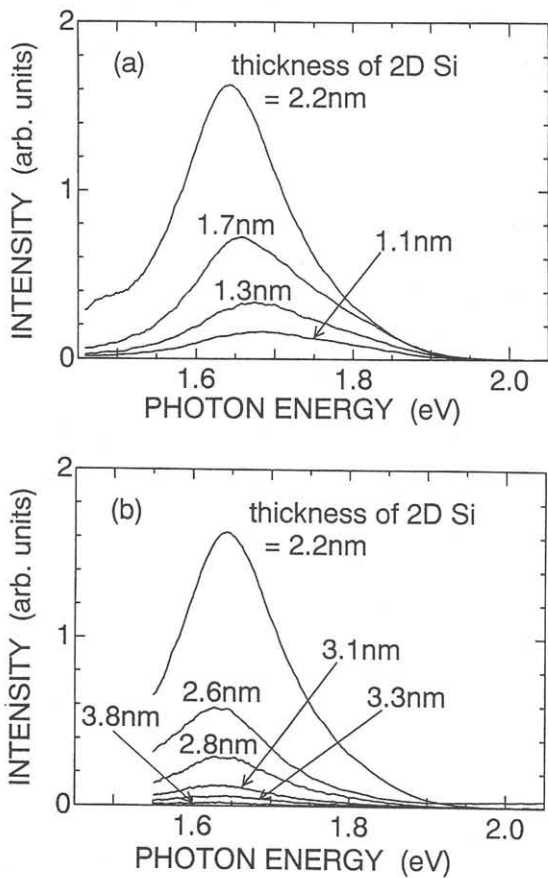


Fig. 2 Photoluminescence spectra at 10 K from 2D-Si (a) thinner than 2.2 nm, and (b) thicker than 2.2 nm.

a function of the Si layer thickness. In this figure, the dotted line indicates the pseudodirect bandgap energies calculated from Eq. 1 (given later). All the spectra have a peak at around 1.65 eV, while a slight peak shift to a higher energy is observed for Si thickness below 2 nm. The fact that the peak energy of the spectra is almost independent of the Si thickness excludes the luminescence mechanism originating from direct recombination in a pseudodirect 2D-Si band.

The peak energies of the spectra shown in Fig. 2 are surprisingly close to the PL from porous Si and Si nanometer-sized spheres (1D or 0D structure).¹⁻⁴ This fact strongly suggests that the luminescence mechanism of the 2D-Si structure is similar to that in a 1D or 0D structure. In fact, our results are consistent with a three-region model proposed by Kanemitsu et al.⁴ in which excitation of electron-hole pairs occurs in the Si well but luminescence originates in the radiative recombination center in the interfacial layer between the Si and SiO₂ layers, as shown in Fig. 4. It should be noted that, in this model, the physical substance of the interfacial radiative center is obscure and hypothetical.

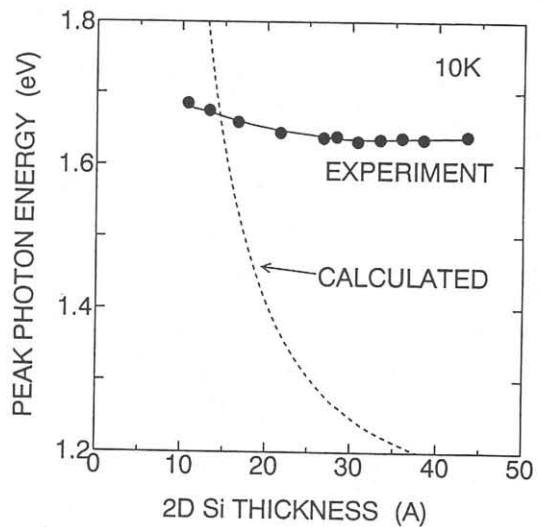


Fig. 3 Thickness dependence of the peak energy of the PL spectra. The dotted line shows the calculated pseudodirect bandgap energy of 2D-Si.

PL peak intensities are plotted in Fig. 5 as a function of the Si thickness. This result can also be explained with the three-region model. As the 2D-Si thickness decreases, PL intensity increases since the 2D energy bandgap (E_{g2D}) in the Si quantum well exceeds the interface state energy for the radiative recombination. Here, the 2D subband serves as the level at which an electron-hole pair transfers to the interface state. Then, further decreases in the thickness cause the PL intensity to decrease because of a decrease in absorption volume and increase in the 2D energy bandgap exceeding the incident photon energy.

Next, the thickness dependence of PL intensity is fitted by the model described above. The effective bandgap energy E_{g2D} of the 2D-Si structure can be estimated by an effective-mass approximation and by assuming the infinite confining potential of SiO₂,

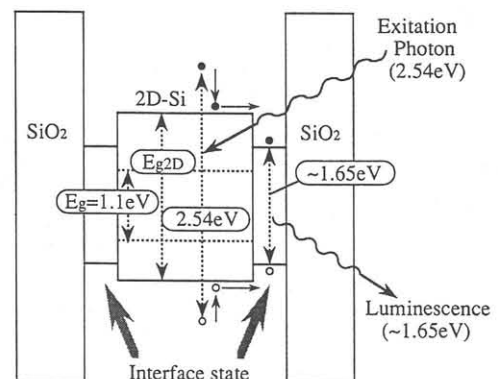


Fig. 4 A band diagram of the three-region model.

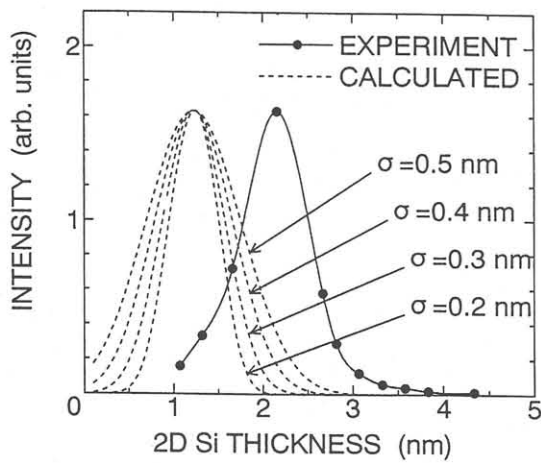


Fig. 5 Peak PL intensity vs 2D-Si thickness. The solid circles and solid line show the experimental data. The dotted lines show the curves calculated under the assumption of Gaussian distribution of the Si thickness.

$$E_{g2D} = E_g + \frac{(\pi\hbar)^2}{2m^* \cdot t^2} + \frac{(\pi\hbar)^2}{2m_{hh} \cdot t^2} \quad (1)$$

where, m^* and m_{hh} are the effective mass of electrons and heavy holes, t is Si thickness, and E_g is the indirect energy gap of bulk Si. To transfer electrons and holes to the interfacial recombination level, E_{g2D} must be larger than the luminescent photon energy of about 1.65 eV. In this argument, relative energy levels of electrons and holes in the Si and the interface are important, but we focus only on the energy gap in both regions for simplicity. On the other hand, the E_{g2D} must be smaller than the excitation photon energy of 2.54 eV. According to Eq. 1, the thickness range satisfying both the photo-absorption and luminescence conditions is $0.9 \text{ nm} \leq t \leq 1.5 \text{ nm}$. Here m^* and m_{hh} are $0.98m_0$ and $0.49m_0$, respectively. The luminescence intensities are calculated as functions of 2D-Si thickness, as shown by the dotted line in Fig. 5. Here, we assume the Gaussian distribution of Si thickness and photo-absorption proportional to the thickness. In this figure, σ is the standard deviation of the Gaussian distribution function. The asymmetric calculation curve fits well the experimental data for a σ of 0.3-0.4 nm if the curve shifts by about 0.9 nm in the thicker direction. These σ values are not inconsistent with the AFM measurement of the Si/SiO₂ interface roughness in SIMOX wafers.⁵ This shift in thickness is due to an offset error in the thickness measurement or band structure modulation through the deformation of 2D-Si lattices caused by the thermal process in 2D-Si formation.

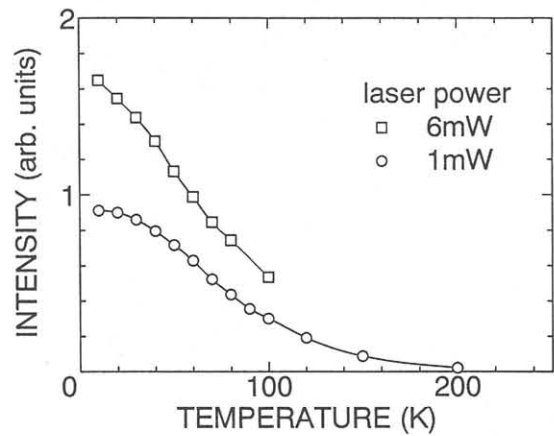


Fig. 6 Temperature dependence of PL intensity of 2D-Si. The thickness of the Si is 2.1 nm.

Figure 6 shows the peak PL intensity from 2.1-nm-thick 2D-Si as a function of temperature. In the temperature dependence of PL intensity in porous Si or Si nanometer-sized spheres (1D or 0D structure), the intensity has a peak at around 50-150K.^{2,4} In the case of 2D-Si, the intensity increases monotonically as temperature decreases. It is likely that confinement only in the one-dimensional direction weakens the localization of excited carriers, resulting in the reduction of the nonradiative Auger recombination process.⁶

4. SUMMARY

We observed PL from a 2D-Si structure on a SIMOX wafer and found a strong dependence of PL intensity on the 2D-Si thickness and thickness-independent PL peak energy which can be interpreted with the three-region model. In addition, we found a different temperature dependence of PL intensity from that found in 0D or 1D structures.

REFERENCES

- 1) L.T.Canham, Appl. Phys. Lett. **57**, 1046 (1990).
- 2) X.L.Zheng, W.Wang, and H.C.Chen, Appl. Phys. Lett. **60**, 986 (1992).
- 3) P.B.Fischer, K.Dai, E.Chen, and S.Y.Chou, J. Vac. Sci. Technol. **B11**, 2524 (1993).
- 4) Y.Kanemitsu, T.Ogawa, K.Shiraishi, and K.Takeda, Phys. Rev. **B48**, 4883 (1993).
- 5) M.Nagase, T.Ishiyama, and K.Murase, Proc. 6th Int. Symp. SOI Technology and Devices, 191 (The Electrochemical Society, Pennington, 1994).
- 6) V.N.Abakumov, and V.I.Perel, and I.N.Yassievich, Nonradiative recombination in semiconductors, (North-Holland, Amsterdam, 1991).