Manifestation of the Quasi-Direct Recombination in Nanocrystalline Silicon Dots by Reducing the Core Diameter

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Recently, the influence of quantum confinement on the optical properties of semiconductor nanostructures is one of the intensively studied fields. For example, the widening of the band gap is due to the smaller dimensions of the nanostructures. Although the breakdown of the **k**-conservation rule due to the strong quantum confinement has been theoretically expected,[1,2] quantitative results related to the breakdown have not been presented yet. For the indirect band gap semiconductors such as Si, the optical transitions are allowed only if the phonons are absorbed or emitted to conserve the crystal momentum. When the size of the Si nanostructures is reduced small enough to relax the **k**-conservation rule, the probability of the quasi-direct recombination increases. The emission from the Si nanostructures is considered on the basis of a competition between indirect and quasi-direct recombinations. Thus, Si nanostructures can be good candidates for the study of the **k**-conservation rule breakdown. We prepared the nanocrystalline Si (nc-Si) dots with the core diameter ranging from ~9 nm to ~4 nm, which is smaller than the exciton Bohr radius of Si, 4.9 nm, while keeping the dot density constant. The room temperature photoluminescence (PL) measurements were performed to observe the quasi-direct recombination in the nc-Si dots.

The nc-Si dots with the core diameter of 9±2 nm, which were prepared by utilizing very high frequency (VHF, 144 MHz) plasma decompositionn of SiH_4 diluted by Ar [3], were deposited on Si (100) substrates for PL measurements. PL spectra of the nc-Si dots oxidized at 750 ˚C for 0 hour and 8 hours are illustrated in Fig. 1 (a) and (b), respectively. Note that the 800 ˚C oxidation was performed for 10 minutes before 750 ˚C oxidation in order to fix the nc-Si dots on the substrates. PL spectra of the nc-Si dots showed in Fig. 1 can be decomvoluted into three gaussian curves (denoted as P1, P2, and P3). P2 emission is originated from the nc-Si dots.[4] The area ratio of the P2 is plotted as a function of the core diameter of the nc-Si dots in Fig. 2. The area ratio drastically increases as $\sim r^{-6}$ with reducing the core diameter r when the core diameter is less than the exciton Bohr radius of Si. Note that the probability of the quasi-direct recombination decays with an approximate $\sim r^{-6}$ behavior.[2] Therefore, the enhancement of the PL intensity of the nc-Si dots can be explained by the manifestation of the quasi-direct recombination in the nc-Si dots due to the strong quantum confinement.

[1] M. S. Hybertsen, *Phys. Rev. Lett.* **72**, 1514 (1994).

[2] M. Iwamatsu, *Jpn. J. Appl. Phys. Part 1* **37**, 5620 (1998).

[3] S. Oda and M. Otobe, *MRS symposia proceeding* No. 358, 721 (1995).

[4] K. Arai, J. Omachi, K. Nishiguchi, and S. Oda, *MRS symposia proceeding*, to be published.

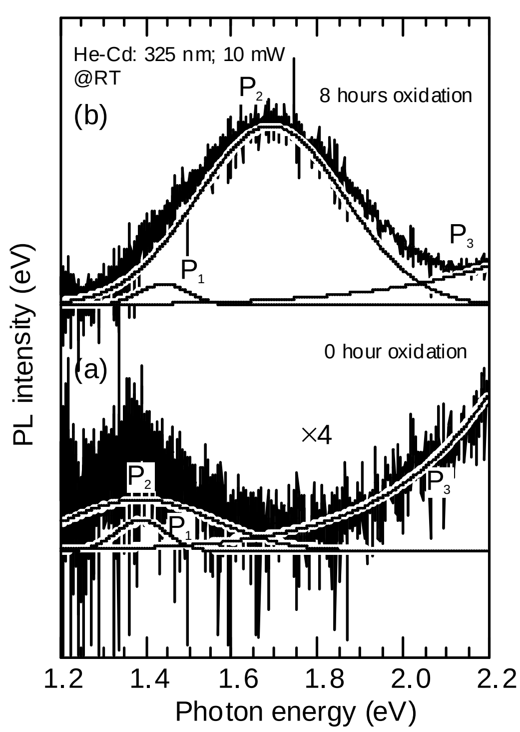

Figure 1: PL spectra of the nc-Si dots oxidized at 750 °C for (a) 0 and (b) 8 hours.

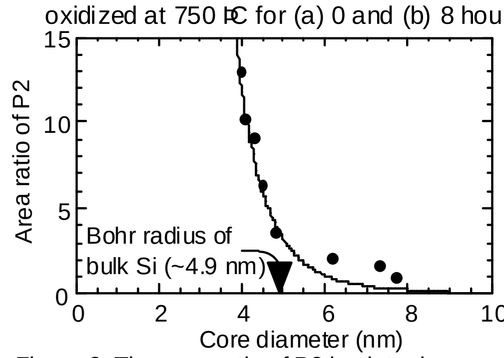

Figure 2: The area ratio of P2 is plotted as a function of the core diameter of the nc-Si dots. A solid curve is drawn as $\sim r^{-6}$.