Enhancement of PL intensity of surface oxidized nanocrystalline silicon dots

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The visible light emission from Si nanostructures has been a subject of focused studies since a decade ago, which will open a door to future devices such as Si-based LEDs and lasers. Although the photoluminescence (PL) of the Si nanostructures is strong enough to be seen by naked eyes, luminescence efficiency of the Si nanostructres is low compared to that of the direct gap semiconductors because of the indirect gap of Si. When the diameter of the nanocrystalline silicon (nc-Si) dot core is less than an exciton Bohr radius of Si of ~4.9 nm, the exciton can no longer exist and an electron-hole pair is generated instead of the exciton. Within the framework of the effective mass model, no-phonon transition will rise when the size of the nanostructure is small enough due to the increase of the overlap integral between the electron envelope function and the hole envelope function [1]. By employing oxidation, the nc-Si dot core with a diameter of sub-5 nm has been achieved [2]. In this study, we demonstrate, for the first time, the enhancement of the PL intensity of the nc-Si dots due to the no-phonon transition with decreasing the diameter of the Si core by oxidation.

The PL spectra of the nc-Si dots oxidized at 750□C for 10 minutes and 8 hours are illustrated in Fig. 1 (a) and (b), respectively. An emission peak is observed in each PL spectrum, which can be deconvoluted into two Gaussian curves (denoted as P1 and P2 in Fig. 1). We discuss here only the P2 peak since it is related to nc-Si. In Fig. 2, the PL intensity area ratio of P2 is plotted as a function of the diameter of nc-Si. The area ratio of P2 is normalized to the area of the 0 hour oxidation sample. The area ratio of P2 increases with increasing the oxidation period. There is an inflection point on the plot at around diameter of 4.5 nm, which is close to the exciton Bohr radius of bulk Si. When diameter is larger than that point, the PL intensity increases slowly with decreasing core diameter. When diameter is smaller than that point, the PL intensity increases drastically with decreasing diameter. The curve in Fig. 2 is fitted to the experimental data by using a function of αa^{-6}, where α is a fitting parameter and a is the radius of the Si core. Because the overlap integral oscillates as a function of the core radius a, and it decays rapidly with an approximate $\sim a^{-6}$ behavior [1]. The fitting curve agrees with the experimental data. Thus, the rapid increase of the area ratio of P2 can be explained by enhancement of the no-phonon transition caused by the decrease of diameter of nc-Si dots.

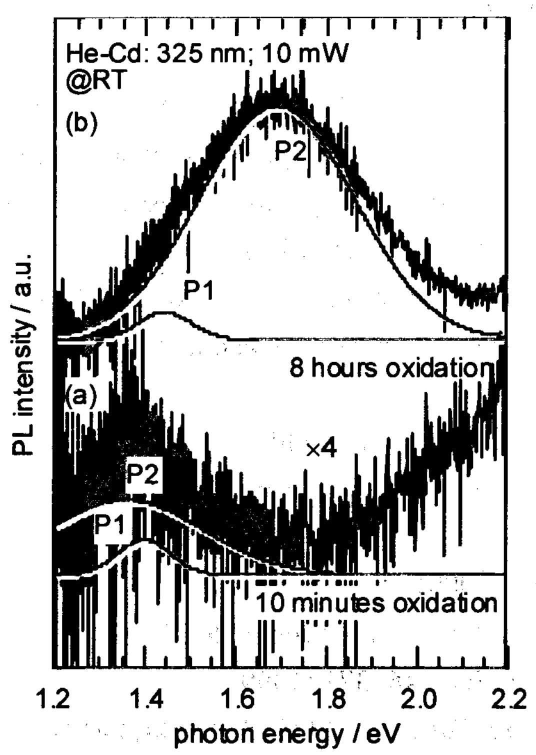

Figure 1: PL spectra of nc-Si dots oxidized at 750□C for (a) 10 minutes and (b) 8 hours.

References

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

[2] J. Omachi, R. Nakamura, K. Nishiguchi, and S. Oda, Proceeding of the Materials Research Society (2000 fall meeting), to be published.

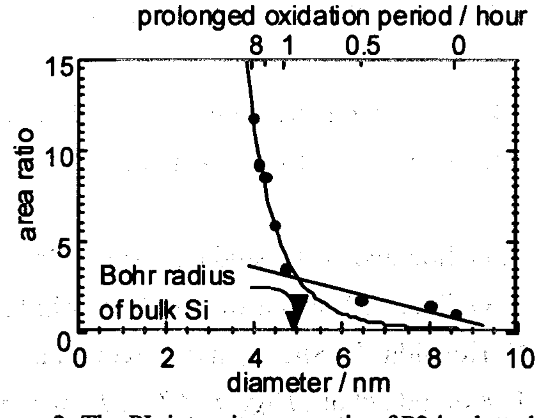

Figure 2: The PL intensity area ratio of P2 is plotted as a function of diameter of the Si core. The oxidation period is also shown.