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Role of ballistic transport in photoluminescence excitation of Si nanocrystals

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Abstract

Photoluminescence of Si NCs with the size (10–300 nm) bigger than the exciton Bohr radius in the bulk Si crystals (4.8 nm) has been considered. Photoluminescence in such NC systems is analyzed from the point of view of new concept based on the effect of hot carrier ballistic transport in excitation of suboxide defect-related photoluminescence at the Si/SiO$_x$ interface. The dependence of the 1.70 eV PL band integrated intensity on Si NC sizes was numerically calculated on the base of the hot carrier ballistic PL model. The well correlation between calculated and experimental results has been obtained for Si NCs with the size from the 30–150 nm range.

Keywords: Silicon; Nanocrystals; Optical spectroscopy; Atomic force and scanning tunneling microscopy; Scanning electron microscopy; Modeling and simulation; Nanoparticles; Optical properties; Luminescence

1. Introduction

The interest on Si nanocrystals (NCs) was stimulated by the discovery of bright red photoluminescence (PL) of porous silicon (PSi) at the room temperature in earlier 1990th of the last century. Numerous scientific publications were issued with results of the photoluminescence (PL) investigation of Si NCs in different types of matrices [1–5]. However up to now the mechanism of bright red PL of PSi is still under discussion as well as the advantages (or disadvantages) of the application of Si NCs in optoelectronic light emitting devices are not clear.

Joint investigations of optical absorption and PL spectra of PSi with different size NCs (2.0, 3.5 and 9.0 nm) have shown a gradual increase in the optical absorption coefficient near the absorption edge when the Si NC size decreases [4]. At the same time no significant size dependence of PL peak energy was observed. Latter the size dependence of peak positions of infrared (1.4–1.6 eV) PL band has been revealed for Si NCs embedded in the SiO$_x$ [5,6]. But the intensity of this PL band was very low and essentially less than intensity of the red PL band in PSi [6].

As a rule two groups of Si NCs have to be discussed. The first group deals with Si NCs of small sizes ($a \leqslant a_B$, where a_B is the exciton Bohr radius equal to 4.8 nm for the bulk Si). PL in such NCs is connected with optical transitions between localized electronic states formed due to the strong quantum confinement effect. The second group deals with NCs of the big size ($a > a_B$) from the range of 10–300 nm. Last case is known as the weak quantum confinement regime and PL for these NCs is controlled by the hot carrier ballistic effect [7]. The paper presents the comparison of PL intensity dependences, obtained experimentally in PSi and numerically calculated on the base of hot carrier ballistic PL model [3,7], versus Si NC sizes from the range of 30–300 nm.

2. Experimental details

PSi layers were prepared as described earlier in [3,6,7]. The size of Si NCs has been estimated using the JSM-T20 (JEOL) scanning electron (SEM) and Nanoscope

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IIIa atomic-force (AFM) microscopes and then it is compared with earlier results obtained by the Raman scattering method [8]. PL spectra were excited by the 3.68 eV N_2 laser line or by the 2.40 eV Ar ion laser line. PL spectra at 300 K were registered using the IKS-12 spectrometer with two detectors for different spectral ranges [3,6]. All PL spectra were corrected on setup spectral response.

3. Results and discussion

PL spectra of PSi samples prepared at different technological conditions are presented in Fig. 1 for two excitation regimes. PL bands peaked at 1.70 and 1.90–2.00 eV have been revealed, which are characterized by different dependences on excitation light energy. Actually the 1.70 eV PL band intensity increases, but the 1.9 eV PL band intensity decreases, with the change of excitation energy from 2.40 to 3.60 eV.

AFM images of PSi layers prepared at different etching current densities are shown in Fig. 2. Table 1 presents the integrated intensity of both visible PL bands and the average size of Si NCs in studied PSi estimated by AFM and SEM methods.

As one can see the 1.7 eV PL band does not change its peak position versus Si NC sizes (Table 1). The intensity of the 1.7 eV PL band varies none monotonically with NC sizes and exhibits a maximum at the value equal to 38.4–40.0 nm (Table 1 and Fig. 1). The highest intensity this PL band approaches at excitation light energy of 3.60 eV. This light is absorbed in the depth of 100 nm mainly, which is comparable with PSi surface roughness and Si NC sizes on PSi surface. The intensity and peak position of the 1.9–2.0 eV PL band vary with Si NC sizes, surface area and oxidation [7]. As we have shown earlier in [3,7] the 1.7 eV PL band deals with suboxide related defects at the Si/SiO_x interface and the 1.9–2.0 eV PL band is associated with defects in the silicon dioxide layer on Si NC surface.

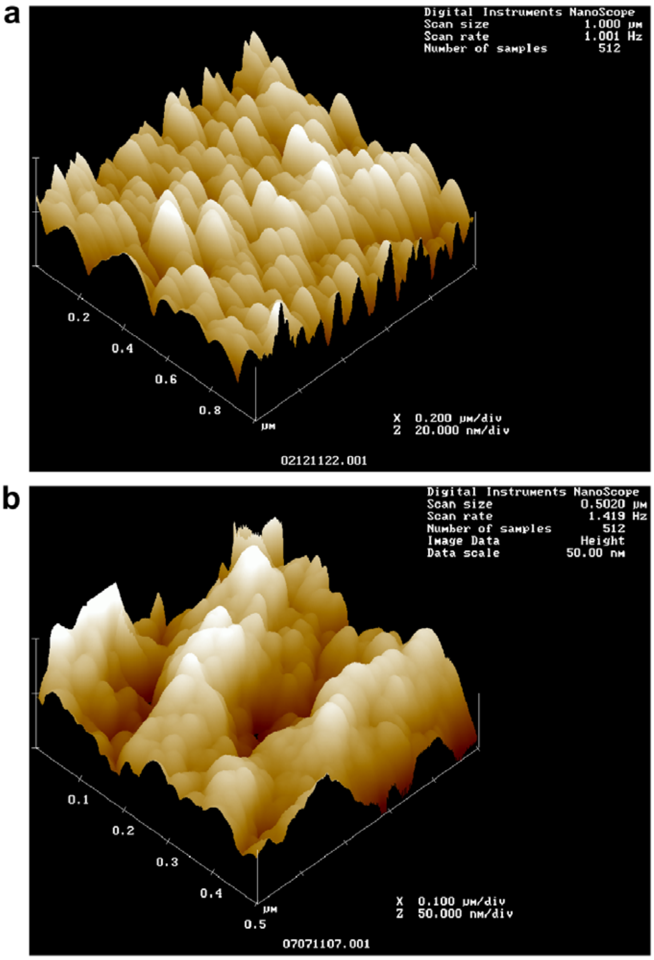

Fig. 2. AFM images of PSi layers prepared at time duration 10 min and etching currents 25 (a) and 75 (b) mA/cm^2.

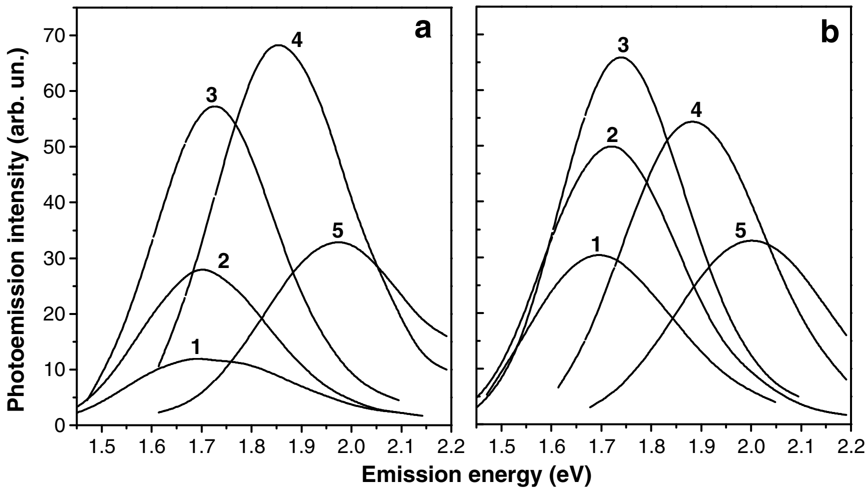

Fig. 1. PL spectra of PSi layers prepared by etching process using the current densities: 5 (1), 10 (2), 25 (3), 50 (4) and 75 (5) mA/cm^2 and duration 10 min, measured at the two excitation energies: 2.40 eV (a) and 3.60 eV (b).