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Manipulation of electronic states and photonic states in nanosilicon

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ABSTRACT

On different size hierarchy, period symmetry provides energy band structure, and symmetry breaking produces localized states in gap, for example nanostructures open electronic band gap by confining electrons, but defects in symmetry system produce localized electronic states in gap. The experimental results demonstrate that controlling localized states in gap by changing passivation environment can manipulate emission wavelength, such as stimulated emission at 700 nm due to oxygen passivation and enhanced electroluminescence near 1600 nm due to ytterbium passivation on nanosilicon. In same way, modulating filling fraction and period parameters in photonic crystal enlarges width of photonic band gap (PBG) by confining photons. Symmetry breaking due to defects is effective in manipulating photonic states. New applications for selecting modes in nanolaser and for building single photon source in quantum information are explored by manipulating and coupling between electronic states and photonic states.

It is interesting in natural sciences that many analogous structures and properties occur on different size hierarchy, for example in nanoscale space related to the de Broglie wavelength of electron and in sub-micrometer scale related to the de Broglie wavelength of photon. Low-dimensional nanostructures for confining electron open band gap and breaking symmetry due to their defect produces localized electronic states in band gap. In same way, modulating filling fraction and period parameters in photonic crystal for confining photon can enlarge width of photonic band gap (PBG). Symmetry breaking due to defects in the lattice is effective in manipulating photonic states. These researches could find some important applications such as a selecting modes device in nanolaser or a single photon source for quantum information [1–8].

For exploring new application of these effects in nanolaser, at first the stimulated emission is obtained on silicon quantum dots (Si QDs) embedded in oxide or nitride, whose wavelength could be manipulated into the window of optical communication by depositing Yb on Si QDs, in which the quantum confinement (QC) effect and the curved surface (CS) effect play main roles [6]. And then a suitably tailored dielectric environment around Si QDs is required for manipulating photonic states [9,10]. Photonic crystals provide resonant cavities for selecting modes of nanolaser, in which it is essential to design crystal structures with PBG as large as possible and to make defect states localize in PBG for coupling the emission [11,12]. In this interesting way, new application in obtaining single photon source is explored, in which single QD for coherent emission is selected by marking on Si QD with characteristic localized states rather than by limiting space for selecting QD. It is fine and novel that defect states localized in PBG is manipulated to couple single QD. In previous work, the CS effect is often submerged in the size effect, which makes some confusion when the QC effect fails for smaller QDs. In manipulating width of PBG, the arising question is for the photon confinement effect and the lattices symmetry breaking effect how to affect photonic states, respectively. In the article, it is a goal to establish the origin and exact mechanism for manipulating electronic states and photonic states on Si QDs and in Si photonic crystals.

Si QDs, embedded in oxide or nitride, are prepared by pulse laser etching (PLE) and pulse laser deposit (PLD) on silicon in various conditions [8]. The laser for PLE is focused on a wafer of P-type silicon placed in nitrogen or oxygen atmospheres. The intensity of the laser pulse is about 5×10^8 W cm^{-2} on silicon, which is sufficient to produce the plasma vibrating on silicon. Nanostructures are prepared by plasma vibrating to distribute on the wall of the Purcell cavity. Then PLD process builds nitride or oxide layer on the nanosilicon. After rapidly annealing and quenching, the structures with Si QDs embedded in nitride or oxide layer are formed by aggregating of rich silicon.

Photoluminescence (PL) spectra of the samples can be measured under the 514 nm excitation at room-temperature by using RENISHAW Micro-Raman Systems. The sharp PL peaks are observed on samples prepared in nitrogen or oxygen atmospheres, which are kept at some wavelength which is independent on sizes of QDs. It is exciting that they have the threshold behavior and the optical gain on samples [13]. Fig. 1 shows the emission coming from localized states in band gap, in which the stimulated emission center at 693 nm (Fig. 1(a)) may be due to Si=O bond and at 604 nm (Fig. 1(b)) is possible coming from

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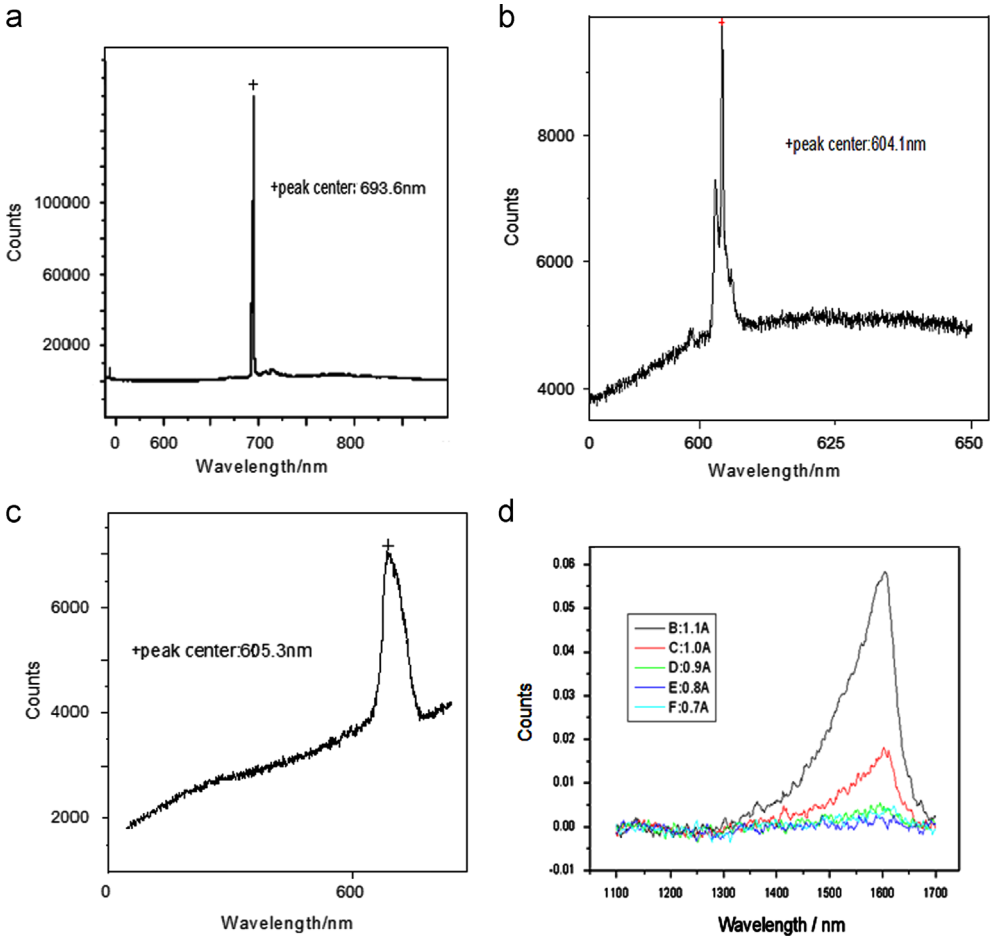

Fig. 1. Manipulation for emission wavelength in PL and EL spectra due to localized states. Stimulated emission at (a) 693 nm and (b) 604 nm for Si QDs prepared in oxygen atmosphere; (c) 605 nm for Si QDs prepared in nitrogen atmosphere; and (d) 1600 nm for Yb deposited on Si QDs prepared by PLD.

Si–O–Si bond on surface of Si QDs. Fig. 1(c) shows a stimulated peak at 605 nm produced from the emission center in nitride layer on Si QDs. The electroluminescence (EL) peaks in optical communication window are observed on the samples in which the Yb ions beam is deposited on Si QDs by PLD, as shown in Fig. 1(d) whose inset indicates that the emission intensity increases with elevation of the pumping current, in which the threshold is about 0.9 A on the sample.

For explaining the emission from localized states, some special surface structures including a facet and a curved surface are built on a Si QDs to compare their density of states. An opened bandgap and a quasi-direct gap structure are obtained for a good passivation of Si–H bonds. Fig. 2(a) shows a Si–Yb bond on the surface with larger curvature, which can provide the localized levels in band gap. But a Si–Yb bond on the facet of Si QDs cannot provide any localized level in gap, as shown in Fig. 2(b). This comparison shows the CS effect on Si QDs. It is clear that larger bond angle on surface of nanostructures related to larger curvature is important to form and manipulate localized states.

In Si QDs system, the level of the electronic states localized in band gap is stated by followed form [6]:

$$E_L = C/r^m - \beta A \tag{1}$$

where β is the bond coefficient, r is the radius of QD and C is the coefficient of QC effect, in which the index m is about 1.7 for Si QDs embedded in oxide. The factor A coming from the simulation calculation involves the surface curvature and the surface systematization as followed: $A = B^{1/(1+d)}/R$, which affects the energy level localizing in gap, where R is the curvature radius of surface, B is the bonding cover factor on surface and index d is cover dimension, such as $d=0$ for S=O bond, $d=1$ for Si–O–Si bridge bond and $d=2$ for Si–N bond or Si–Yb bond. They relate to point, line and film forms of bonding cover on surface, which determine the level position of the localized states in gap. In the formula (1), the first term relates to the QC effect for confining electrons, and the second term presents the CS effect for breaking symmetry from abrupt larger curvature on bonding place of Si QD, which provides the localized levels in band gap. Here, the CS effect obviously brings symmetry breaking in the QD system.

The calculation in the CS effect model for breaking symmetry of Si QD demonstrates an interesting relationship between the energy levels localized in band gap and the bonding angles on surface with different curvatures, for example some Si–O–Si bond with different bonding angle on curved surface produces localized state with different level in band gap. As shown in Fig. 3, it is clear that the smaller bonding angle related to larger surface curvature makes the shifting of localized states to deeper position in band gap on Si QD. It is useful in this way for the states gap ΔE to be manipulated into the window of optical communication by the CS effect.

The CS effect is often submerged in the size effect when the diameter of QDs is smaller than 3 nm [14]. In physical conception the QC effect depends on sizes of Si QDs because of confining electron to increase energy which is described by the first term in the formula (1), but the levels of the localized states slowly arise along with the second term in the formula (1) on smaller Si QDs with sphere shape. As shown in Fig. 4, the QC effect and the CS effect for Si–O–Si bridge bond on spherical QDs are compared, in which the different trends in evolution occur. The elevating of the