

A Hybrid Model of Silicon Nanowires

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Abstract

Computer simulation using matlab programming approach is carried out to study the photoluminescence (PL) properties of silicon (Si) nanowires (NWs) with diameter between 1.5 and 5.8 nm. An integrated hybrid model comprising of quantum confinement, surface states, and exciton binding is developed to calculate the size, wavelength and photon energy dependent PL intensity. The influence of size on the band gap energy and PL spectra of Si nanowires (NWs) are examined. It is observed that all the model parameters for quantum confinement, localized surface states, and exciton energy are responsible for the changes in the electronic and optical properties of Si NWs. The simulated data are compared with experimental findings. The admirable features of the results suggest that the present model is significant for understanding the mechanism of visible PL from Si- NWs. The model can be extended to study temperature dependent PL for other nanostructures of different shapes and size.

Keywords: Photoluminescence; quantum confinement; nanowires; passivation; radiative recombination

1.0 Introduction

Developing novel electronic and optoelectronic devices by nanostructuring semiconductors is ever-demanding. The observation of room-temperature visible photoluminescence (PL) from silicon (Si) nanostructures (quantum dots or wires) stirred tremendous attention towards Si nanomaterials [1]. It is their great properties like electrical and optical that make them to receive such attentions. Recent semiconductor research is exploring the feasibility of tuning the optical response of Si nanostructures via band gap engineering. Growth direction, morphology, size and surface reconstruction also influence the luminescence properties of SiNWs [2]. Experimentally observed visible PL can be explained to some extent by quantum confinement (QC) effect that modifies the energy band gap [3]. Lately, Si nanostructures with hydrogen and oxygen passivated surface became attractive due to enhanced light emission. However, the mechanism of visible PL remains unclear despite several studies using models, experiments, and simulations approaches [3 – 5].

An analytical model for silicon nanocrystals (Si NSs) photoluminescence of quantum confinement effect and localized surface state have been proposed by Ding et al. [6] and Estes and Moddel [7]. In this work, we developed a comprehensive phenomenological/hybrid model by combining the effects of surface states, exciton energy, and QC to explain the PL mechanism of Si NWs. These combined three phenomena of quantum confinement, surface passivation and exciton effects which determine the optoelectronic properties of Si NWs is what makes this proposed model a unique from the other proposed models mentioned earlier. It is demonstrated that by controlling a set of parameters extracted by fitting the model with experiments, it is possible to interpret the PL spectral features accurately. The band gap is found to decrease with the increase of NWs diameter [8]. The results presented here allow us to examine the influence of size on the band gap energy and PL spectra of Si nanowires (Si-NWs).

2.0 Models and Methods

The initial and the famous explanation for the visible PL in Si-NWs is the quantum confinement of exciton in nanometer-sized silicon. The model of the quantum confinement of Si NWs is based on the electronic confinement in wire. An empirical

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law that links the size dependence of optical band gap of NWs is written as:

$$E_g = E_g^{bulk} + \frac{b}{d^\delta} \tag{2.1}$$

where b and δ are QC parameters and d is the diameter of Si-NWs [9].

The model is further fitted with different experimental and simulation data to extract the value of this parameter. Because of quantum confinement, small-diameter wires exhibit a direct band gap that increases as the wire diameter narrows, irrespective of surface termination. The photoluminescence is attributed to energy shift of the bottom of the conduction band to high energy and of the top of the valence band to low energy [10]. The changes in wave functions explaining the dynamics of electrons and holes that modifies the density of states is due to different in quantum confinement directions.

In this model, we consider Si- NWs of well defined diameter distribution as an ensemble of nanoscale spherical particles. In view of this consideration, the intensity of PL at particular photon energy becomes proportional to the population of occupied surface states and the oscillator strength. The number of surface states in a crystallite is proportional to the number of atoms on the surface and hence, surface area A of the crystallite. If N_t is the total number of surface states then $N_t \propto A$. Again, if we assume that each atom in a crystallite contributes at least one photo excited carrier to the crystallite, the number of photo excited carriers N_p in a crystallite is proportional to its volume V , hence, $N_p \propto V$. Furthermore, since the rate of transition from an excited carrier to the localized surface states is proportional to the product of the number of excited photo carriers and the number of available empty surface states in steady state condition, the population N_c of photo carriers in surface states participating in PL processes becomes proportional to the product of N_t and N_p . That is,

$$N_c \propto N_t N_p \propto d^2 d^3 \tag{2.2}$$

where d is the diameter of the crystallites wire.

The rate of radiative transition depends on the oscillator strength f . The oscillator strength in nanocrystalline materials varies as inverse power law and can be approximated as $f \sim 1/d^\alpha$, where power exponent α depends on the material properties as well as the range of crystallites sizes being used. Taking the oscillator strength into account, the radiative transition probability in a nanocrystallites of diameter becomes,

$$P(d) \propto N_c f \propto d^{5-\alpha} \tag{2.3}$$

The PL intensity from an ensemble of crystallite of Si NWs having size distribution will be obtained by summing the contributions from all the crystallites having size diameter d [11]. The PL intensity with respect to crystallites of size d is given by,

$$I(d) \propto P(d)\rho(d) \tag{2.4}$$

Then, the emitted photon energy from nanocrystallites wire will be lower than the energy band gap of the crystallite by an amount of the localization energy E_{ss} of the surface states and the exciton binding energy E_{ex} which are functions of crystallites size. The emitted photon energy from crystallites of the quantum dot is given as

$$E_p = E_g^{bulk} + \Delta E - E_{ss} - E_{ex} \tag{2.5}$$

where the amount of band gap up shift due to QCE in the nanocrystallites wire is given by ΔE and E_g^{bulk} is the energy band gap corresponding to the bulk crystalline material. By transforming Eq. (2.4) from d to ΔE dependence by a standard procedure (Fourier Transform), we obtain

$$I(\Delta E) = \int I(d) \delta\left(\Delta E - \frac{b}{d^\delta}\right) dd \propto \int d^{5-\alpha} \rho(d) \delta\left(\Delta E - \frac{b}{d^\delta}\right) dd \tag{2.6}$$

By considering a normal distribution of crystallite diameters in nanocrystallites silicon wire, then

$$\rho(d) = \frac{1}{\sigma\sqrt{2\pi}} \text{Exp}\left[-\frac{(d-L_0)^2}{2\sigma^2}\right] \tag{2.7}$$

where L_0 and σ are the mean crystallite size of NWs and standard deviation, respectively. Substituting Eq. (2.7) into Eq. (2.6), we obtain the analytical expression of PL intensity as

$$I(\Delta E) \sim \frac{1}{\sigma\sqrt{2\pi}} \left(\frac{b}{\Delta E}\right)^{(6-\alpha+\delta)} \text{Exp}\left[-\frac{\left\{\left(\frac{b}{\Delta E}\right)^{\frac{1}{\delta}} - L_0\right\}^2}{2\sigma^2}\right] \tag{2.8}$$

Eq. (2.8) indicated that the PL profile varies strongly with the QC parameters b and δ . Therefore, good care should be taken in using the correct QC model for band gap up shift estimation. The oscillator strength and the exciton binding energy E_b both are complicated functions of the size of nano crystallites and their surrounding media. Following careful calculations of Proot *et al.* [12] for crystalline silicon, we adopted a ranging value of 0.01 - 0.22 eV for E_b , which is a good average value for the range of crystalline sizes from ~ 5.8 nm to 1.5 nm. The localization energy E_{ss} is taken to be the order of phonon energies which is about 0.05eV for optical phonons and E_g as 1.12 eV for crystalline silicon at room temperature [12].

The orientation dependent parameters are found to be $b = 1.40$ and $\delta = 3.37$ eV. This is obtained by fitting the model with experimental values of size dependent band gap of Bruno *et al.* [13] using quantum electronic gap expression (Eq.2.1) as shown in Figure 1. Our model expression (Eq.2.8) is used to generate PL spectra using these quantum confinement parameters with the correction of ± 0.5 for comparison and further analyses [14]. PL spectra are simulated using a matlab program. The band gap energy is found to increase as the NWs diameters are decreased.

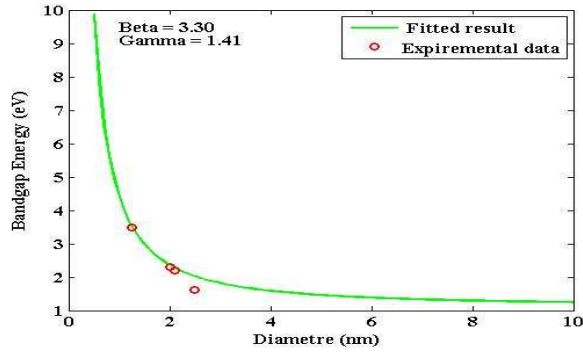


Fig. 1. Band gap variations of Si-NWS with diameter.

3.0 Results and Discussion

PL intensity versus photon energy with varying standard deviation is shown in Figure 2. It indicated that the PL peak shift towards higher energy (blue energy) as the silicon nanowire standard (sigma) deviation parameters decreases. This validated the quantum confinement model. Furthermore, a red shift is observed with the increase of standard deviation σ . The PL spectra broaden as well as shifts towards low photon energy accompanied by a decrease in relative PL intensity. This indicates that the amount of size dispersion affects both the PL peak energy and its width.

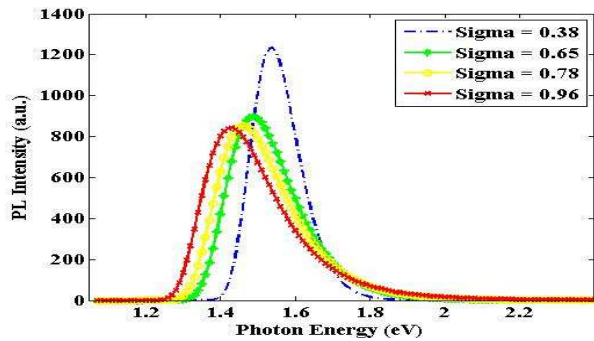


Fig. 2. Simulated PL spectra for Si nanowires having size distribution with fixed mean diameter, $L_0 = 3.80$ and different standard deviation.

It is clear from Figure 2 that the presence of exciton energy in the forbidden region contributed for the observed blue shift. Hence, the integrated surface states effect, exciton states, and quantum confinement effect model can explain accurately the experimentally observed PL spectra of Si NWs and the blue shift in PL peak [15].

Definitely, this model is able to predict the already observed experimental PL data on Si NWs produced by a variety of techniques. Figure 3 compares the simulation results (right) with the experimental (left) data from Ledoux et al. [11]. Clearly, a blue shift in the PL peak is evidenced with the decrease in mean diameter of Si NWs. Furthermore, the PL intensity is greatly influenced by the size distribution (L_0) of NWs.

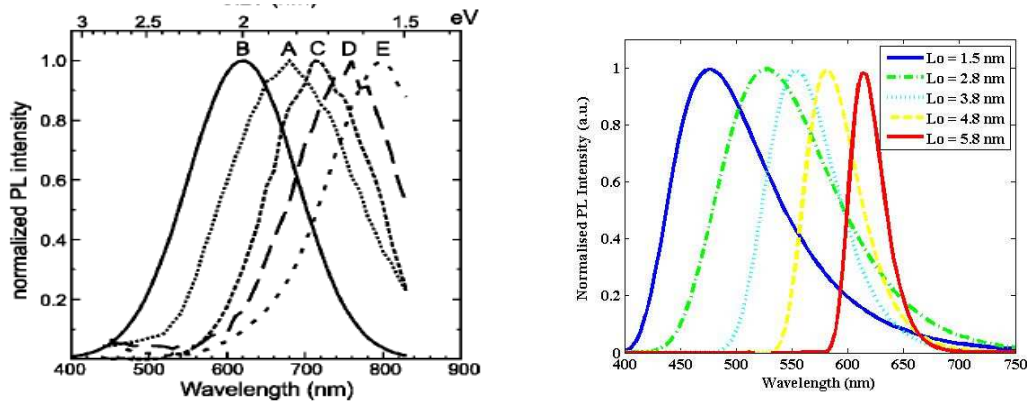


Fig. 3: Normalized PL spectra against wavelength from experiment (left) and model simulation (right).

4.0 Conclusion

The mechanism of photoluminescence and the enhancement of band gap in SiNWs are investigated using a hybrid phenomenological model. The effects of quantum confinement, localized surface states and exciton binding energy are integrated in the model. Unlike in other proposed models of luminescence, exciton binding energy plays a good role in enhancing the quantum confinement effect in SiNWs such that the enhanced radiative recombination rate of excitons occurs only with decrease in nanowire size that result in bandgap widening. The results exhibit that by controlling a set of parameters extracted by fitting this developed model with experimental finding, it is possible to interpret the observed PL spectral features. It is shown, how mean diameter of NWs affects the PL intensity and band gap energy. We affirm that both QC and surface passivation together with exciton effects determine the optoelectronic properties of Si NWs. The mechanism of PL emission and enhancement of band gap is understood. In general, this developed model is able to explain the experimental observation of visible PL from Si-NWs as well as others Si nanostructures (quantum dots and wells).

5.0 References

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