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Full Length Research Article

# A MODEL STUDY OF SURFACE STATE ON OPTICAL BANDGAP OF SILICON NANOWIRES

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**ABSTRACT**
A theoretical approach is carried out to study the role of surface state in silicon nanowires. The influences of size and surface passivation on the bandgap energy and photoluminescence spectra of silicon nanowires with diameter between 4 to 12nm are examined. It is observed that visible PL in silicon nanowires is due to quantum confinement and surface passivation. But the energy recombination of electron and holes in the quantum confined nanostructures is responsible for the visible PL. In this work, models from quantum bandgap and photoluminescence intensity are adopted to explain the size dependent surface luminescence. Investigation show that the nanowires of smaller size with surface impurities revealed higher bandgap energy. Oxygenated surface is found to have higher energy than hydrogenated surface. The features of PL spectra of Si nanowires suggest that these models are significant for understanding the mechanism of visible PL from SINWs.

**Keywords:** Photoluminescence, Surface State, Band gap, Quantum Confinement

## INTRODUCTION

A nanocrystal made of semiconductor material is now an interesting means of new electronics and optoelectronics devices, and it has become predominantly significant over last two decades (Vasiliev et al., 2001). The huge efforts made toward matter manipulation at the nanometer scale have been motivated by the fact that desirable properties can be generated by just changing the material dimension, morphology and shape (Kanemitsu, 1995). In particular, silicon nanowires (NWs) are attracting attention from the electronics industries due to their demand for small devices, from cell phones to computers etc. The discovery of room temperature visible PL from porous silicon and Si nanostructure (Canham, 1990) and possibility of tuning the optical response of silicon nanosized material by modifying their size has invited several attentions in these special kinds of nanoclusters and in small semiconductor structures (Bruno2007). It is found that unlike bulk silicon which has indirect bandgap, the nanostructure Si have direct bandgap and emit light from violet to red depending upon the size of nanostructure (Ghoshal et al., 2014).

The role of surface defect need to be understood for the utilization of nanostructured silicon nanowires (SINWS) for possible application in electronic and optoelectronic devices. In addition the correlation between the defects and the optical properties, it is also noticed that at nanoscale, the size not only directly impacts the defect contents but also the optical properties of materials (Harrison 2005). Optical and electronic properties of SINWS are controlled by surface effect and quantum confinement. Recently, passivated surface Si nanostructures with hydrogen and oxygen become attractive due to enhanced luminescence observed in them. Geometry plays a crucial role in the enhanced surface defect due to large surface-to-volume ratio (Ghoshal, 2005). Light emitting surface of Si nanometer size crystallites faded by hydrogen and oxygen atoms which differentiate the electronic properties of the near-surface region in the crystallites from those of the crystal-silicon core in the crystallite (Matsumota et al., 1993).

The mean diameter of SiNWs has been shown to have an effect on the PL intensity and bandgap energy (Ghoshal et al., 2012). We present here the effect of quantum confinement on optical bandgap in silicon nanowires of different sizes and the role of hydrogen and oxygen surface on the optical properties of nanostructures. Both oxygenated and hydrogenated surfaces are used for examining the passivation effect. A developed model of quantum bandgap energy and photoluminescence intensity are used to determine the role of size and surface state, and is able to predict both already published simulation PL (including pseudo-potential approximation and tight binding method) data and experimental PL data on silicon nanostructures produced by a variety of techniques. The importance of localized surface states in predicting the PL data from SiNWs using the developed models are demonstrated.

## SIMULATION METHODOLOGY

Visible luminescence origin in SiNWs is based on quantum confinement effect and surface state effect (Kanemitsu, 1995 and Ghoshal et al., 2007). Here, we considered the quantum confinement and photoluminescence intensity models to make semi-empirical fittings with the other simulations findings and generate PL spectra. The model of quantum confinement of SiNWs depends on the electronic confinement in wire. An empirical law links the size dependence optical bandgap of NWs as (Ghoshal et al., 2014);

$$E_{gap} = E_{gap}^{bulk} + \text{Þ}/d^{\gamma} \quad (1)$$

Where Þ $\boldsymbol{and}\ \boldsymbol{\gamma}$ are quantum confinement (QC) parameters and d is the diameter of NW. Because of the QC, small diameter wires exhibit a direct band gap that increases as the wire diameter narrows, irrespective of surface termination. The size confinement in different directions also changes the wave functions describing the behavior of electrons and holes that modifies the density of states (Ghoshal et al., 2014). Later, we fit this model with the pseudo-potential approximation and tight-binding methods simulation data of Ghoshal et al. (2005) to extract the values of parameter Þ $\boldsymbol{and}\ \boldsymbol{\gamma}$ and study the variation of bandgap energy with surface passivation. These extracted values of QC parameters with the correction of ± 0.5 are used to generate PL spectra using general expression for PL intensity profile from nanocrystal silicon (NC-Si) ensemble in Eq. (2). 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 Ă of the crystallite. The PL intensity profile is;

$$\boldsymbol{I}(\in) \sim \frac{1}{\sigma\sqrt{2\pi}} \left(\frac{\text{Þ}}{\in}\right)^{\frac{6-\alpha+\gamma}{\gamma}} \boldsymbol{exp}\left\{-\left[\left(\frac{\text{Þ}}{\in}\right)^{\frac{1}{\gamma}} - \boldsymbol{L_o}\right]^2 / 2\boldsymbol{\sigma}^2\right\} \quad \textbf{(2)}$$

With ∈ as the amount of bandgap up-shift due to size confinement in nanocrystallites, $\boldsymbol{and}\ \boldsymbol{L_o}$ and $\boldsymbol{\sigma}$ are the mean crystallite size and standard deviation respectively. Eq. (2) generally depend strongly on size confinement parameters Þ $\boldsymbol{and}\ \boldsymbol{\gamma}$. we compared carefully the calculations of Proot et al. (1992) for crystalline silicon in getting the ranges values of parameters used in the intensity profile above.

## RESULTS AND DISCUSSION

Data from size dependent band gap of Tight Binding Theory and the Pseudo Potential Approximation method are fitted with quantum electronic gap in Eq.(1) as shown in Fig. 3.1 and 3.2. The Þ $and\ \gamma$. values of the quantum confinement parameters for PPA are found to be 10.5 and 1.39 and for TBM it is 13 and 1.39, respectively (Ghoshal et al., 2005). The band gap energy is found to decrease as the NWs diameter is increased at high diameter. There are a small percentage of surface atoms, while at low diameter; there is an appreciable percentage of surface atoms and vice versa. The results show that surface defects play a huge role in influencing the band gap widening in SiNWs. Oxygenated passivated surface is found to increases more than the hydrogenated surface. The quantum parameters found from the fitted energy are used to generate PL spectra of nanocrystalline-Silicon structure using a MATLAB programming.

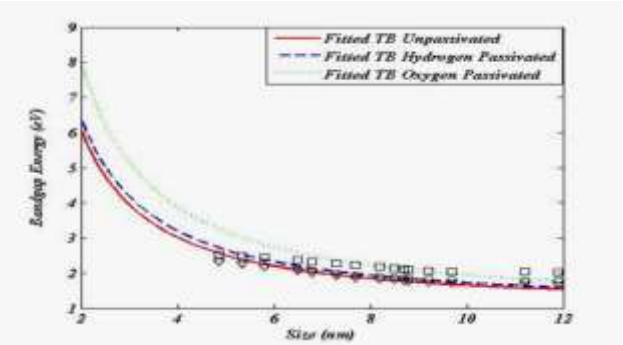


**Fig 3.1:** Fitted gap energy from pseudo potential model

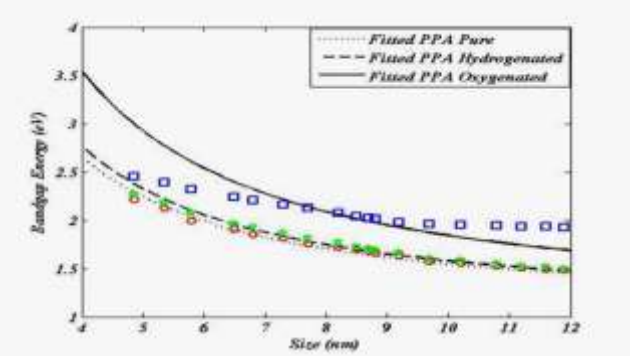


**Fig 3.2:** Fitted gap energy with the one obtained using tight binding model

Figure 3.3 and 3.4 present PL spectra generated using parameters found from size depended band gap (PPA and TBM).The PL peak profile distributions in fig. 3.3 reveals how luminescence size dependence surface state behaves .The results indicated that surface passivation enhances the band gap energy of the nano-Si structure and also provides conformity with a surface state effects..

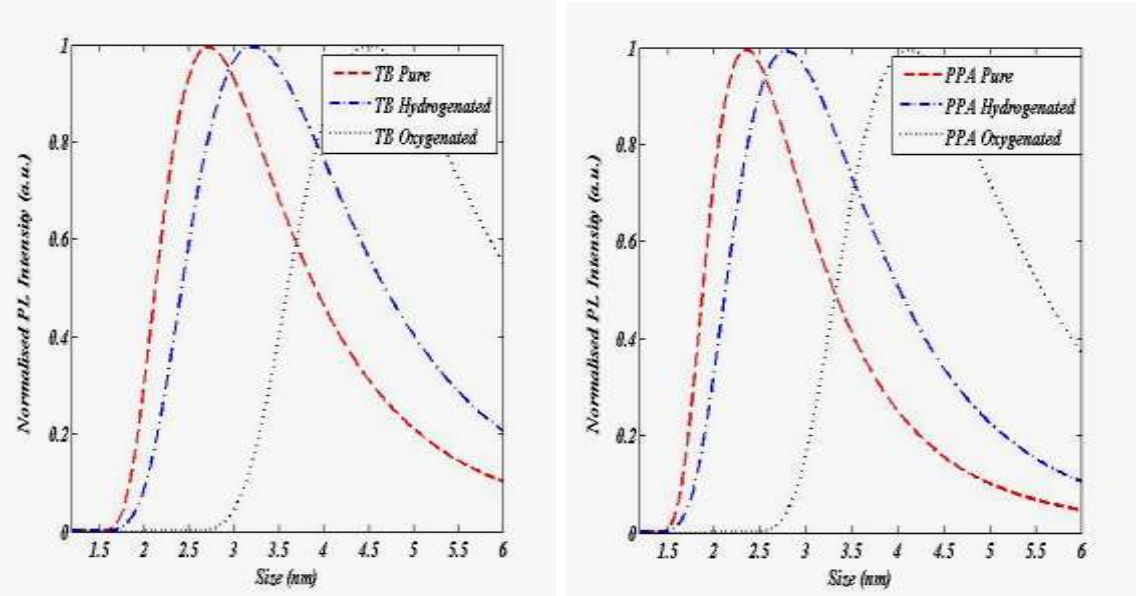


**Fig 3.3:** NWs diameter dependent PL Spectra from Tight binding model and Pseudo potential approximation

The photon energy dependent PL profile in fig.3.4 provides details on how the PL peak is shifted toward higher energy as the surface of SiNWs become passivated

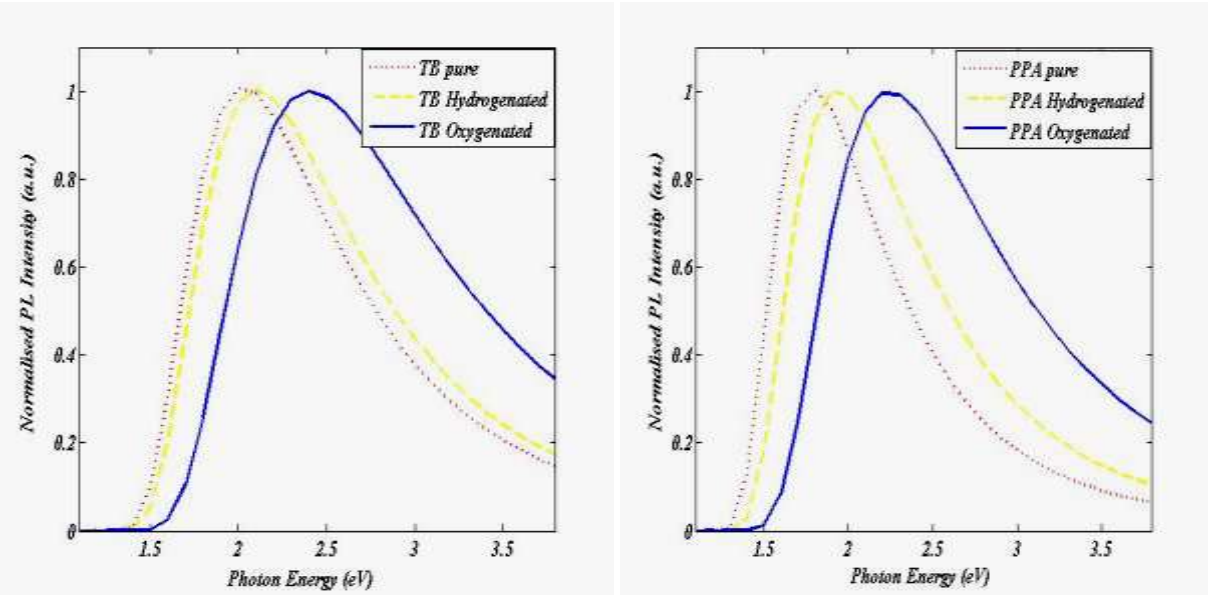


**Fig 3.4:** Photon energy dependent PL Spectra from TBM and PPA

**Conclusion**

Quantum confinement effects, localized surface states and exciton binding energy are used in the combined model to describe simulation (PPA and TBM) data PL spectra and the enhancement of surface band gap from silicon NWs. The mean diameter of Si NWs has been shown to have an effect on the PL intensity and band gap energy. The role of surface passivation for NWs of diameter 1.5-6nm on the band gap and PL intensity is demonstrated. The mechanism of PL emission and enhancement of band gap is understood. Both oxygenated and hydrogenated surfaces are used for examining the passivation effects. The developed model and the extracted parameters highlighted the effect of confinement and surface on the PL emission from Si NWs. In general, the importance of localized surface states in predicting the PL data from Si NWs using the developed models are demonstrated. This study is in conformity with other model calculations and theoretical predictions. However it is important to look at multiple distributions of crystal sizes (which dictate the band gap variation) to get a better estimate of visible PL. The result obtained can be utilized as a clue to control the luminescence properties in device production..

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