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**Research Article**

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# A Model Study of the Influence of Temperature on the Photoluminiscence of Silicon Nano Cryatals

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**Abstract** The influence of temperature on photoluminescence (PL) intensity of silicon nanocrystals (SiNCs) is carried out using a theoretical model. A combined model of quantum confinement effects (QCE), surface State effect (SSE), exciton binding energy and temperature dependence band gap expression is developed to examine the temperature dependent PL between 1-3.6 nm of silicon nanocrystals (SiNCs). The model indicate that at the nanoscale the PL peak of the size dependent temperature luminescence is shifted to the smaller size as the temperature increases indicating a blue shift, while PL increases as the temperatures decrease. This implies that at higher temperature, the particles required small amount of energy to cross to the conduction band which reduces the bandgap and that an appreciable luminescence is observed at room temperature, which validate the experimental findings. All the features of the work are estimated by the use of a MATLAB program and are found to be consistent with experimental and other theoretical approaches.

**Keywords** Photoluminiscence, Silicon Nano Cryatals

## Introduction

The possibilities of turning the optical response of silicon nanosized material by modifying their size have invited intense theoretical and experimental investigations in recent years. In the past decades, several breakthroughs have increased the hopes of using nanostructured silicon as an optical active material. The basic idea has been to take advantage of the reduced dimensionality of the nanocrystalline phase (1-5 nm in size) where quantum confinement, band folding and surface effects play a crucial role [1]. The increased interest in this area of research arose when room- temperature visible luminescence from Si and Ge nanostructures was discovered [2]. It has been found that the band-gap of Si nanocrystals (NCs) increases with decreasing NC size and is accompanied by an efficient luminescence [3]. Nanostructuring silicon is an effective way to turn bulk silicon into a photonic material. It is established that quantum confinement (QC) can modify the energy gap such that visible luminescence is observed as experimentally confirmed [4]. With a large surface- to- volume ratio, the surface effects, and also the quantum confinement effects, control the optical properties of these materials [5].

It has been established that these nanostructures and their porous form have a direct band gap and emit light from violet to red depending upon the nanostructure’s size [6]. Experimentally, it has been confirmed that efficient visible luminescence from silicon nanocrystals are attributed to the transition between confined electron and hole states inside the nanocrystals. Thus, the origin of the visible luminescence mechanism in silicon nanocrystals can be explained to some extend by the quantum confinement effects and the surface state effects [7]. Despite several proposed experimental and theoretical models to explain the phenomenon, including the quantum confinement and the surface state, no conclusive argument has been given yet on the mechanisms of this efficient light emitted from porous silicon, silicon NWs and related semiconductor materials.

The bandgap energy of Si and other semiconductors tends to decrease as the temperature is increased and increase with decrease in the temperature which also affect the photoluminescence. The phenomenon can be better understood if one considers that the inter-atomic spacing increases when the amplitude of the atomic vibrations increases due to the increased thermal energy. An increased inter atomic spacing in turn reduces the size of the energy bandgap.

When the dimension of this material is reduced from bulk to nanoscale its physical and chemical properties like melting and boiling points also change.

In this work we will theoretically examine the influence of temperature on the luminescence of silicon nanocrystals. A model of photoluminescence intensity as a function of temperature, quantum confinement and surface state is develop to determine the effects of the temperature on silicon nanocrystal using a MATLAB program.

## Method and Model

A model of photoluminescence intensity as a function of temperature, quantum confinement effects, and surface state is formulated to investigate the influence of temperature on the optical behavior of silicon nanocrystals.

According to quantum confinement model, the size dependence of optical band gap of NWs is given as

$$E_{g_{nano}} = E_g^{Bulk} + \frac{\beta}{d^{\gamma}}, \qquad (1.0)$$

Where β and γ are quantum confinement parameters, $E_{g_{nano}}$ is the energy gap of the nanowires, $E_g^{Bulk}$ is the energy gap of the bulk silicon and d is the size of the nanowire.

The temperature dependence of the energy gap in semiconductors is given by the Varshni relation as:

$$E_{g(T)}^{Bulk} = E_g(0) - \frac{\alpha T^2}{T+\beta_1}, \qquad (2.0)$$

Where α and $\beta_1$are the constant characteristics of the material, $E_g(0)$ is the value of the gap at 0K temperature and T is the temperature in K. Substituting equation (2.0) into equation (1.0) lead us to

$$E_{g_{nano}} = E_g(0) - \frac{\alpha T^2}{T+\beta_1} + \frac{\beta}{d^{\gamma}} \qquad (3.0)$$

Also the emitted photon energy from Si crystallite is given as

$$E_{PL} = E_g^{Bulk} + \Delta E - E_s - \Delta E_b \qquad (4.0)$$

Where $E_g^{Bulk}$ is the band gap corresponding to the bulk material, ΔE is the amount of band gap upshift due to the quantum confinement effect in the nanocrystallite, $E_s$ is the amount of the localization energy of the surface state and $E_b$ is the exciton binding energy.

∴ combining equation (2.0) and (4.0) gives:

$$E_{PL} = E_g(0) - \frac{\alpha T^2}{T+\beta_2} + \Delta E - E_s - \Delta E_b \qquad (5.0)$$

And hence

$$\Delta E = E_{PL} + E_s + \Delta E_b + \frac{A T^2}{T+\beta_2} - E_g(0) \qquad (6.0)$$

The general expression for PL intensity is:

$$I(\Delta E) \approx \frac{1}{\sigma\sqrt{2\pi}} \left(\frac{\beta}{\Delta E}\right)^{\frac{\sigma-\alpha+\gamma}{\gamma}} e^{\left\{\frac{-[\left(\frac{\beta}{\Delta E}\right)^{\frac{1}{\gamma}} - d_0]^2}{2\delta^2}\right\}} \qquad (7.0)$$

It is clear from the above expression that the PL profile will depend strongly on temperature and the QC parameters β and γ.

In this work a PL intensity against size, wavelength and photon energy as a function of temperature is plotted using a MATLAB program, QC parameters, β and γ are obtained by fitting an experimental work with the model in equation (1.0). All the results obtained will be compared with the other published experimental and theoretical works.

## Results and Discussion

From the experimental work of Hong Yu et al., (2011), presented in Fig.1.0, we used GetData graph Digitizer software and extracted the values of energy gap and diameter from the work and later fitted it with the quantum band gap energy relation in. Eqn. (1.0) to get the quantum confinement parameters Beta β = 3.08 and Gamma γ = 1.26 [8].

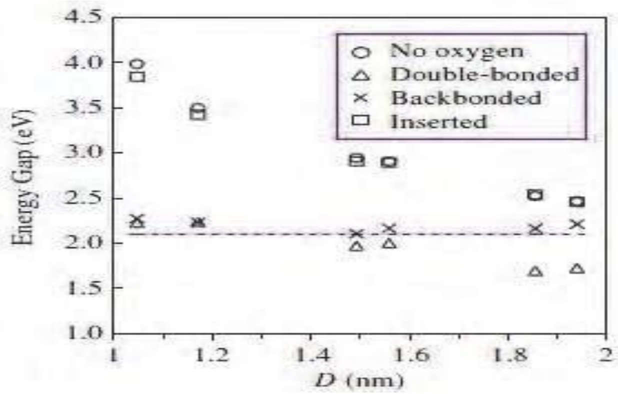

*Figure 1: Energy Gap versus Diameter*

A result of the fitted band gap against size is presented in Fig. 2. The encircled points represent the experimental work of Hong Yu et al.,(2011),while the full line graph gives the fitted energy of Beta β= 3.08eV and Gamma, γ = 1.26. These quantum confinement parameters (β and γ) are used in our developed model to estimate the influence of temperature dependence photoluminescence [8].

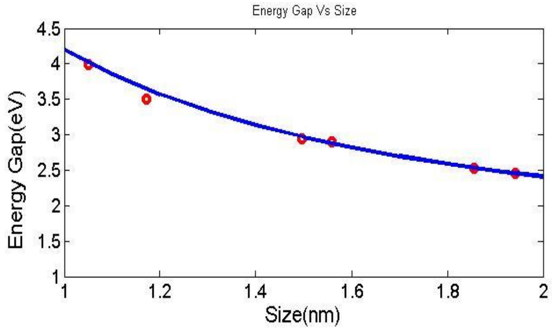

*Figure 2: Fitted Energy Bandgap*

Equation (7.0) is used to simulate the normalized photoluminescence PL against size with varying temperature as shown in Fig. 3. It is observed that PL are strongly dependent on temperatures and size distributions. The PL peak is shifted to the smaller size as the temperature increases indicating a blue shift, while PL increases as the temperatures decrease [9].

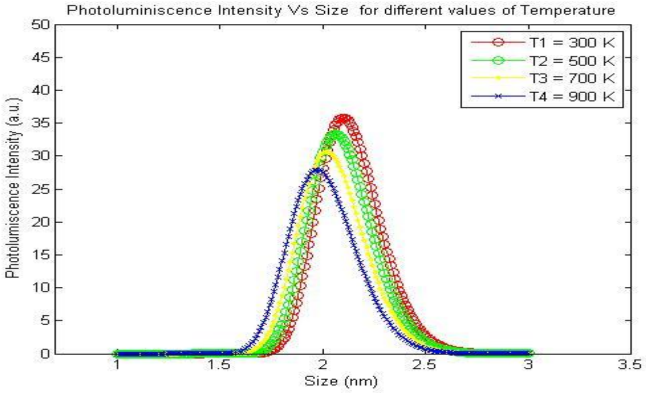

*Figure 3: Photoluminescence Intensity against size (nm) at different temperatures*

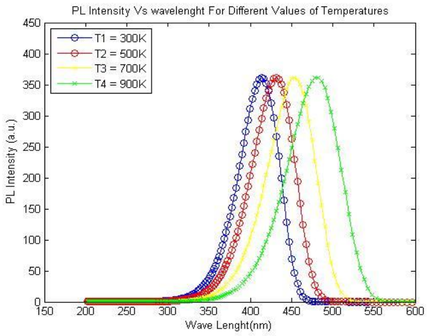

*Figure 4a: Photoluminescence intensity versus Wave length*

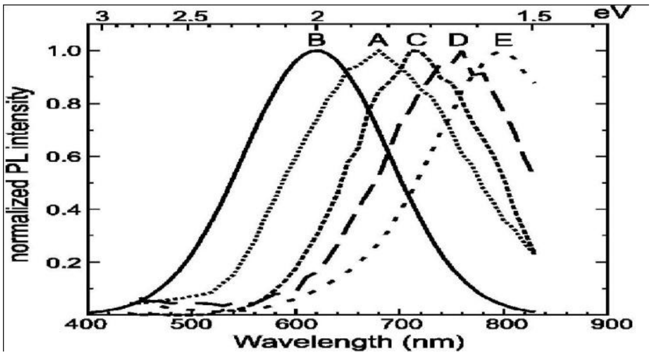

*Figure 4b: Photoluminescence intensity versus Wave length [9]*

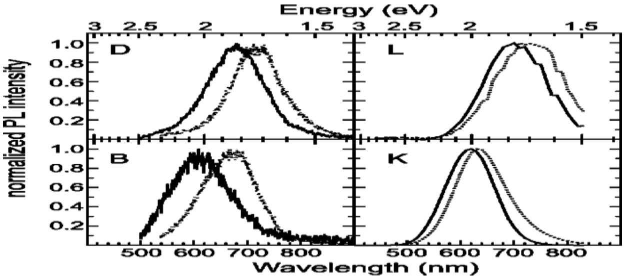

*Figure 4c: PL spectra for four nanocrystalline Si samples (B, D, K, and L) [9]*

The influences of temperature dependent PL spectra are shown in Fig. 4.a as simulated using our developed model. This model is able to predict the already observed experimental PL data on Si NWs by variety of techniques. Figure 4.0a compares the simulation results with the experimental (Fig. 4.b) data from Ledoux et al., (2000). The blue-shift observed in the PL peak is evidenced with the decrease in temperature of the system. The PL intensity is greatly influenced by the temperature of the NWs. On the long wavelength (low energy) side of the graph, the PL intensity shows a blue-shift with decreasing temperature. The PL intensity in the short (visible) wavelength (high energy) range shows the opposite behavior: a red-shift with increasing temperature [9].

The developed model is used to simulate PL intensity against photon energy using MATLAB program, the result of the plot obtained is presented in Fig. 5a. The result is consistent with the experimental works of Ledoux et al., (2000) and (2002) Fig. 5b, as compared. Fig. 5a, gives the various PL peaks as a function of temperatures of the nanocrystals. It can be observed that, coming from lower temperature on the right hand side , the peak of the PL band systematically shift toward the blue (lower energies) when the temperature of the particles is increased. This implies that at higher temperature, the particles required small amount of energy to cross to the conduction band and appreciable photons is observed at room temperature.

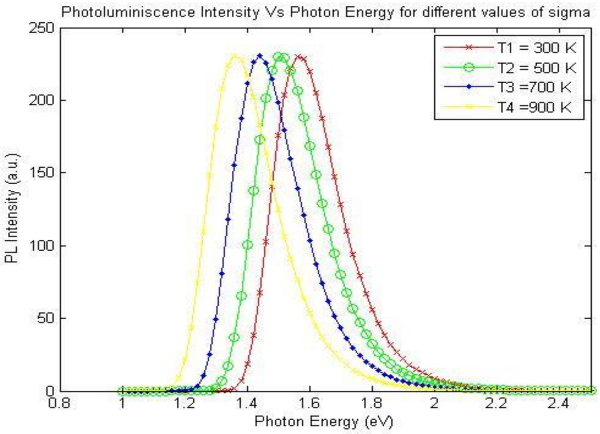

*Figure 5a: Photoluminescence versus Photon Energy*

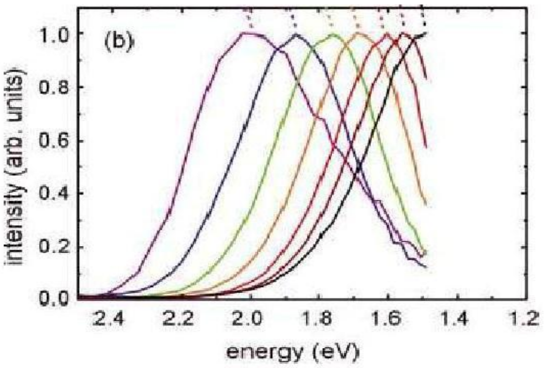

*Figure 5b: Photoluminescence versus Photon Energy [9]*

## Conclusions

The influence of temperature on the PL intensity are investigated using a developed model by deriving an expression for NWs temperature dependent PL intensity and band gap which is used to determine the influence of temperature dependent visible PL against size, wavelength and photon energy.

The results obtained can be well understood since the theorytical variation of PL positions is close to the experimental behavior. Our results reveals that, by controlling a set of parameters extracted when this developed model is fitted with experimental fidings, the observed PL spectral features can be interpreted. The obtained results show how temperature affects the PL intensity in which we observed a blue- shift to the luminiscence with decreasing temperature (low energy, long wavelenght and reduced size) and red shift to the luminescence with increasing temperature (high energy short wavelenght and incresing size). In general, this model is able to explain the experimental observation of visible PL from Silicon Nanocrystals.

We have concluded that the PL intensity of Si NWs strongly depend not only on the size of the nanocrystals, *i.e*. on the quantum confinement and the surface passivation but also on temperature. Our results are in qualitative agreement with other observations as well as with experimental results.

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