ORIGINAL ARTICLE

Electroluminescence from Silicon and Germanium Nanostructures

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Abstract

Silicon (Si) and germanium (Ge) have an indirect band gap transitions; however when they are miniaturized to nanometer scale, the energy gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) increases, and hence the transition changes to direct due to confinement. In this paper we explain photoluminescence (PL) and electroluminescence (EL) and formulate models to study electroluminescence from Si and Ge nanostructures. Using the models we got computational results to explain the dependence of EL on different parameters like size of the nanocluster, applied voltage, band gap energy, and wavelength for pure silicon nanocrystal (Si-nc) and for oxygen and hydrogen terminated Si-nc. The EL and PL intensities occurs at the same energy; however, the EL intensity has sharp Gaussian sub peaks and red shifted compared to the PL intensity. To get our result, we used the idea of quantum confinement model (QCM), that can explain PL and EL on pure Si nanostructures and Si-terminated with impurities.

Keywords: Quantum confinement, Nanostructure, Exciton binding energy, Electroluminescence

INTRODUCTION

It has been realized that the integration of optoelectronic components on all Si matrix would considerably simplify the conception and fabrication of integrated optoelectronic devices, Hirschman et al. (1996). However, Si is a poor light emitter because of its indirect band gap impedes radiative transitions. Its use in optoelectronics is very limited, especially for light emitting devices such as light emitting diodes (LEDs) and solid state (Si) lasers, the latter being a starting point of many optoelectronic devices . Si is widely used in semiconductors because; it remains semiconductor at higher temperatures than the semiconductor Ge and because of its native oxide it is easily grown in furnace and forms a better semiconductor/dielectric interface than any other material, Daniel Miloni (2006).

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Silicon nanowire (SiNW) growth with hydrogen passivation has been demonstrated and extensive experimental and theoretical studies of electronic, optical, and mechanical properties have been performed. SiNWs have a direct band gap, with potential applications in electronic, optoelectronic, and chemical sensors, Daryoush Shiri et al. (2008).

Si is the leading material concerning high density electronic functionality, its band gap (1.12 eV) is ideal for room temperature operation, and its oxide allows a processing flexibility to place large number of transistors on a single chip. However, all the single transistors and electronic devices have to transfer information on length scales which are relevant with respect to their nanometeric scale. In bulk Si competitive non-radiative recombination rates are much higher than the radiative ones and most of the excited electron-hole (e-h) pairs recombine non-radiatively. This yields very low internal quantum efficiency for Si luminescence. As what concerns the lasing of Si, fast non-radiative process such as Auger or free carrier absorption severely prevent population inversion at high pumping rates needed to achieve optical amplification; D. R. Vij (2004), G. G. Ross et al. (2008), Jasprit Singh (2003), Minoru Fujii et al. (1998,) S. Prezioso et al. (2008)].

Many papers are reported regarding PL and EL, nowadays due to the optoelectric properties electroluminescence and photoluminescence from Si and Ge nanostructures are still debatable issues.

METHODOLOGY

In order to obtain the desired result for this work, we have formulated model equations that describe the dependence of PL and EL intensity on the size of the nanocluster. Fourier transform have been employed to transform from size dependent intensity to energy dependent intensity. Matlab program have been developed for the model equations that simulates the data to compare with experimental results. The results obtained with this simulated data with the model equation agree with experimental results done by other researchers. The following section presents the formulated model equations that have been used for developing the matlab code for data simulation.

Formulation of models

There exist two classes of explanation for the origin of the visible PL and EL in P-Si, the quantum confinement effects and the surface state effects. Here we consider the hybrid model mixing them to investigate EL. The quantum confinement model (QCM) is based on the electronic confinement in dot like structure of Si. The development of this model is based on the effective mass approximation theory. In this model, the luminescence process is attributed to an energy shift of carriers (electrons and holes).

Assuming that a Gaussian size distribution about the mean diameter L_0 for the nanocrystallites; for a P-Si sample consisting of varying column diameters the probability distribution of electrons participating in the PL process is:

$$I_{el} = \frac{1}{\sqrt{2\pi}\sigma} bL^2 \exp\left(-\frac{(L-L_0)^2}{2\sigma^2}\right)$$

Where b is a suitable normalization constant. The luminescence intensity can be expressed in terms of energy by taking the Fourier transform from of the above equation as:

$$I(\Delta E) = \frac{bc_1{}^3}{2\sqrt{2\pi}\sigma} \Delta E^{-\frac{5}{2}} \exp\left\{\frac{-L^2{}_0}{2\sigma^2}\left[\left(\frac{\Delta E_0}{\Delta E}\right)^{\frac{1}{2}} - 1\right]^2\right\}$$

where ΔE is the energy shift due to the confinement given by:

$$\Delta E = h\nu - \left(E_g - E_b\right)$$

E_g being the bulk band gap of Si or Ge in this sample and E_b is the exciton binding energy, and $E_0 = \frac{c_1}{L_0^{\,2}} L_0$ being the nanocrystal mean diameter and σ standard deviations. The values of E_g ranges from 1.11 eV to 1.17 eV for Si, depending on temperature; however, we took 1.12 eV for Si and 0.7 eV for Ge which is actually reported in most standard experiments at room temperature, while the value of E_b varies with nanocrystal radius of the sample ranging exponentially from 0.05 eV (r=5 nm) to 0.24 eV (r=1nm). The EL spectrum is caused by injection of strong electric field $\vec{E}$ or current, the energy associated to this field is:

$$E = NZ\left|\vec{E}\right|L$$

where N is the number of nanocrystallite Si or Ge taken in the sample, Z is the number of electrons in each atom, $\vec{E}$ is the external applied electric field responsible for EL, and L is the diameter of the single atom; since EL and PL occurs at the same energy, using the analogy of the PL spectrum model we can write the energy shift in terms of the applied on the nanocrystal sample. According to the QC model, the emission wavelength and intensity depends on nanocrystal diameter, size distribution and concentration. This model can explain the general tendency of most experimental results such as the blue shift of the luminescence spectrum with decrease of the Si-nc size. The QC model is highly predictive when the nanoclusters are isolated from the matrix (e.g; Si-nc isolated from SiO2). Consequently this model does not give a satisfactory explanation for the evolution of the luminescence spectra for some experimental parameters such as the PL for sample temperature below 100K, as well as oxidation or oxygen passivation of samples containing Si-nc. Due to this reason we used
another model for terminated Si-nc.

RESULTS AND DISCUSSION

Using the ideas of the above models and developing matlab programs, we got some results that are academically interesting and fit with experimental explanations. Few results are presented in this paper.

Dependence of PL intensity on wavelength for different σ

The figure below shows the PL intensity as a function of wavelength for both
Si and Ge nanostructures. As we can see from the figure, the PL intensity for both nanostructures seems to be almost similar since they have the same band structure except a slight change in the band gap energy. The standard deviation from the mean crystallite (which in fact contains the dependence of PL intensity on size) influences on the intensity. Putting different values of sigma suppresses the nature of the luminescence intensity that would have been on the smaller value of sigma in the spectrum.

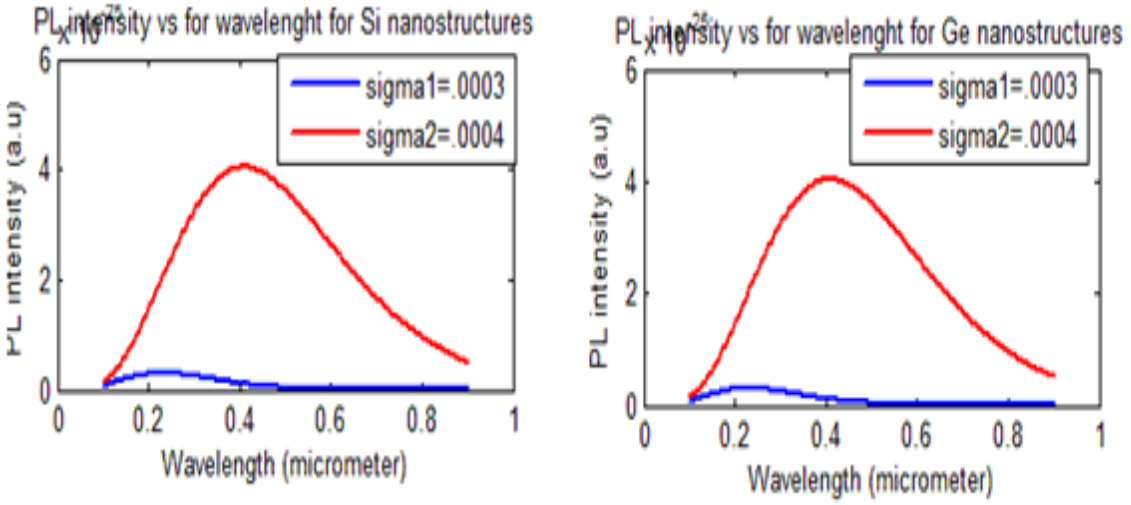

Figure 1: Dependence of PL intensity on wavelength: the left graph is for Si nanostructures and the right one for Ge nanostructures.

This is as expected because the PL intensity depends on the emitted photon energy, not to the number of emitted photons.

Dependence of EL intensity on wavelength for different σ

Fig. 2 shows the dependence of EL intensity on wavelength for both Si and Ge nanostructures. The figure shows most properties observed in PL intensity.

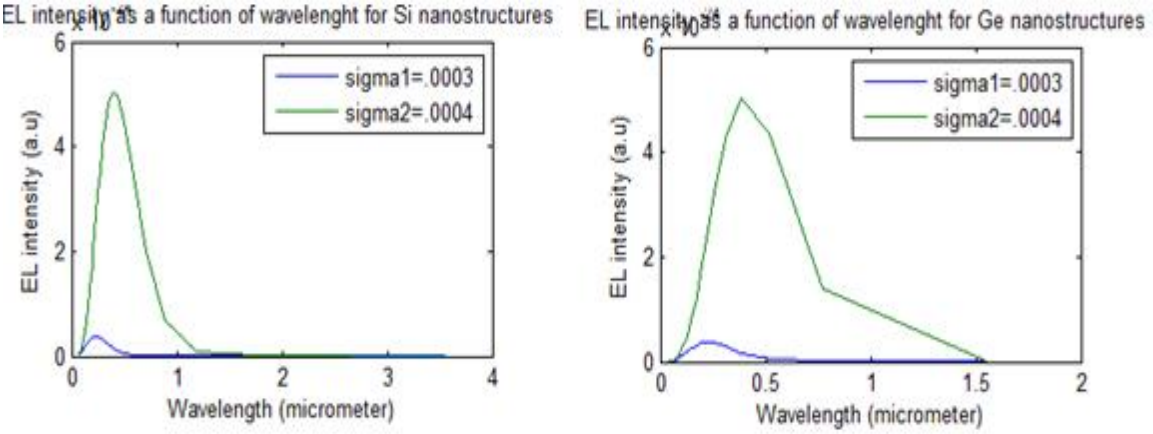

Figure 2: EL intensity as a function of wavelength: the left graph is for Si nanostructures and the right one for Ge nanostructures.

The results of fig. 1 and fig. 2 are computational, however they still agrees with many experimental reports, K. V. Shcheglov et al. (1996).
If we do for single sigma, the nature of the curve looks like exactly the same as the result of experimental curve. When we compare fig.1 and fig.2 it seems that the EL spectrum and the PL spectrum have the same luminescence center, but the EL intensity has sharper peak than the PL intensity this is so because of high contribution for PL intensity from non-radiative recombination channel compared to its contribution for EL.

EL intensity and voltage
The EL intensity increases as the voltage applied to the nanocluster increases; yet to have a spectrum in the visible range we need to select the appropriate range of values of voltage.

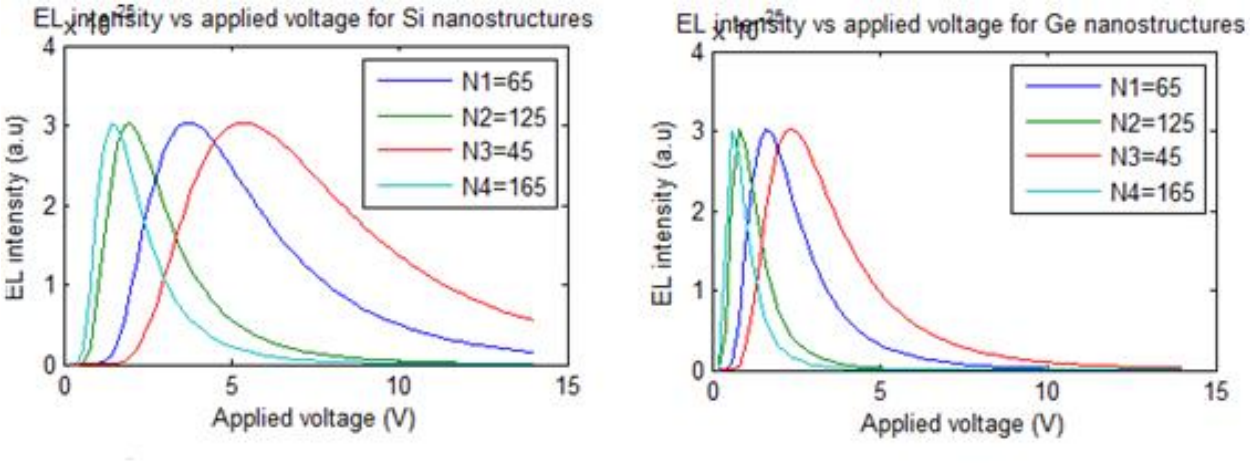

Figure 3: EL intensity as a function of applied voltage: the left graph is for Si nanostructures and the right one for Ge nanostructures.

As the applied voltage increases the EL intensity increases, this does not mean that high voltage is needed for visible EL spectrum; low voltage (<6 V) is needed for good quantum efficiency and visible EL spectrum. The spectral characteristics shows that EL is red shifted compared to PL, while PL is blue shifted compared to EL. Termination of Si with oxygen induces a blue shift in the EL and PL spectrum. The EL spectrum shape is similar to the PL one showing that the two phenomena have the same origin, namely recombination of carriers confined in to the crystallite.

Summary and conclusion

QC effect is more prominent in Si and Ge nanostructures, its effect is the enhancement of radiative recombination rate of excitons with decreasing the cluster size; it also increases the band gap. PL and EL spectrum are caused by optical and electrical excitations respectively. Both have the same luminescence center and occurs at the same energy; however, the EL spectra has more narrow Gaussian sub peaks and red shifted than the PL spectra. A blue shift to the luminescence is observed with decreasing nanocrystal size. Visible light emission in Si becomes possible with radiative recombination rates.

The light generated by e-h recombination in Si and Ge nanostructures is quantified by quantum efficiency.

Generally the HOMO-LUMO gap determines the energy of emitted photon spectrum, the intensity of this spectrum depends on the size of the nanocluster and the energy shift due to confinement. The EL intensity depends on applied voltage, current density, temperature, time, size, and nature of the nanocluster sample taken. It is observed that the power efficiency is very sensible to the applied voltage, and low voltage (<6 V) is necessary to obtain high efficiency and visible EL spectrum. EL always shows either reversible or permanent degradation with time, stability of EL intensity can be improved by termination of Si with O or H. EL spectrum is independent of the applied injection current; however the EL intensity increases linearly with the applied injection current density.

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