

# Dielectric Reduction of Nanometric Amorphous Silicon

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**ABSTRACT** Theoretical values of in amorphous silicon quantum dots (1.8 – 12 nm) dielectric reduction have been calculated. These calculations presented that the dielectric constant of amorphous silicon quantum dots is suppressed. Also, it has been investigated the frequency dependence of the dielectric constant. The variation of the dielectric constant with frequency is similar to the variation of polarizability and polarization. The dielectric constant is made up of contributions from electronic, atomic, and space charge polarization. With the presented calculations, the effect of quantum confinement was adopted, since the bandgap of nano semiconductors can be governed by the size of amorphous silicon quantum dots.

**Keywords:** dielectric constant, dielectric suppression, amorphous silicon, photoluminescence, nano semiconductor.

## 1. INTRODUCTION

When the semiconductor is miniaturized until the nanometer scale, that tendency will produce an expansion in the bandgap ( $E_G$ ) [1]. It gives rise to the blue shift in the photoemission and photo-absorption edges of nanometric semiconductors and the inner energy levels of the core band shift towards higher binding energy [2]. Because of bandgap expansion, the dielectric constant of a nanometric semiconductor is no longer keeping constant but it is significantly suppressed with decreasing of dot size [3]. This will lead to the blue shift in photoabsorbance, where the dielectric constant of nano semiconductors decreases with decreasing of dot size. The reduction of the dielectric constant can also enhance the Coulomb interaction among electrons, holes, and ionized shallow impurities in nanometric devices, as well as the increase in the energies for exciton (electron-hole pair) in nanometric semiconductors due to the reduction of dielectric constant. The dielectric constant value decreases with increasing the incident photon energy on the semiconductor.

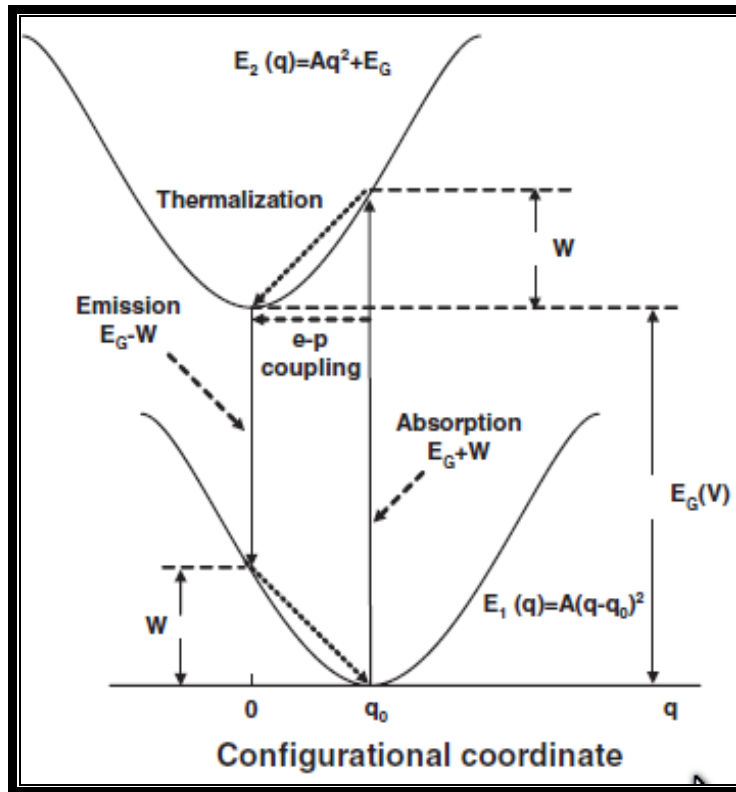
This subject has fund less attention to the investigation of how the change in dielectric constant is affected with the nanostructure semiconductors. Therefore, it is very interesting to build a model to satisfy the reduction in the dielectric constant of semiconductors in the case of the nanostructure.

## 2. THEORY

In this work, the electron-phonon (e-p) interaction contributes to the processes of photoemission  $E_{PL}$ , photo-absorption  $E_{PA}$ , photoconduction, and electron polarization that dominate the static dielectric constant [4]. The PL or PA energy does not represent the bandgap but they are determined by the joint effect of crystal binding and electron-phonon coupling [4]. Figure (3-1) shows the influence on el.-ph. reaction and binding energy to crystal on energy for the photoluminescence  $E_{PL}$  and photo-absorption  $E_{PA}$ . Parabola forms were expressed for the ( $E_1$ ) that is ground state and the ( $E_2$ ) that is excited state [5]:

$$\begin{cases} E_1(q) = E_v(q) = A(q - q_0)^2 \\ E_2(q) = E_c(q) = Aq^2 + E_G \end{cases} \quad (1)$$

The configurational coordinate which is functioned by both the energies of the ground state  $E_1(q)$  and the excited state  $E_2(q)$ , that is the dimension of wavevector. The shape of the parabolas was limited by the constant  $A$ . The interatomic distance is adversely proportion with the  $q_0$ , where  $d_i: q_0 \propto d_i^{-1}$  [6]. The energy gap ( $E_G$ ) represents the perpendicular displacement of the two minimum for the conduction and valence bands that depends exclusively on the crystal potential. The electron–phonon interaction was arisen the lateral displacement  $q_0$ , that can be reinforcement by boost lattice constriction. Hence, the electron–phonon interaction and the crystal binding energy will contributes mutually to the blueshift in the photo absorption and in the photoemission. The magnitude of lattice vibration and frequency are affected by the atomic coordination number diminution and boost bond increase at a surface. Therefore, the electron–phonon interaction will boost the Stokes shift at the surface [7].



**FIGURE(1):** Schematics to photoluminescence  $E_{PL}$  and photo absorption  $E_{PA}$  for nano semiconductor, including binding energy to crystal ( $E_G$ ) and e–p interaction ( $W$ ) [8].

There are three steps that arise in which process. First, absorbing a photon excites an electron with energy equal to  $E_G + W$  from the minima ground state into an agitated state with the generation of pairs from holes and electrons. Second, a thermalization experience of the excited electron leads to moves to the minima of the excited state. Third, electron transfer to the ground state and combines with the hole. The release of a photon relates to the carrier recombination, with energy equal to  $E_{PL} = E_G - W$ . The law of energy and momentum conservation must be applied in the processes of the generation and recombination of the carrier. The absorption energy for photon or the variation in the energy between the higher agitated state  $E_2(q)$  (conduction band  $E_C(q)$ ) and the lesser ground state  $E_1(q)$  (valence band  $E_V(q)$ ) at  $q$  is specific as [5,6]:

$$\begin{aligned}
 E_c(q) - E_v(q) &= \hbar\omega = E_2(q) - E_1(q) \\
 &= (Aq^2 + E_G) - [A(q - q_0)^2] \\
 &= E_G + 2Aqq_0 - Aq_0^2
 \end{aligned} \tag{2}$$

$$= E_{PL} + 2Aqq_0 \tag{3}$$

Where  $\hbar$  represent Planck's constant,  $\omega$  is the frequency and  $E_{PL}$  is the energy of photoluminescence.

The absorption for EM waves is constant scripty the imaginary part for the dielectric constant  $\epsilon_r'(\omega)$  that is liable to the energy lack of the falling waves by the transition of electrons from VB to CB [63, 68], specified by [9 – 11]:

$$\epsilon_r'(\omega) = \frac{F}{\omega^2} \int \frac{f_{cv}}{|\nabla_q [E_c(q) - E_v(q)]|} ds \tag{4}$$

Where  $F$  is a constant,  $s$  is the variant of the area between two bending surfaces in space of *wave vector* for higher and the lesser bands and  $\nabla_q$  the gradient in  $q$  space.  $E_c(q)$  and  $E_v(q)$  match to energies in the VB and the CB in reciprocal space at  $q$ .  $f_{cv}$  is the probability of the transition between subbands, which deferent disregard with the size of particle in the approximation of first order. The alteration of size-induced for transmission probability between the sublevels is almost no mention of small.  $f_{cv}$  is taken as constant, and is usually of the order of unity [10].

Meet the energy and momentum conservation must be exist when integration around a wave vector  $q$  surface. The gradient and the area of elemental to integral are deduced as [12]:

$$\nabla[E_c(q) - E_v(q)] = 2Aq_0 \tag{5}$$

$$ds = 2\pi q_0 dq \tag{6}$$

Substitute equation (5) and equation (6) in equation (4) we get

$$\epsilon_r'(\omega) = \frac{\pi F f_{cv}}{A\omega^2} q \tag{7}$$

By inserting equation (3) into the relation(7) we get

$$\epsilon_r'(\omega) = \frac{\pi F f_{cv} \hbar\omega - E_{PL}}{2A^2 q_0 \omega^2} \tag{8}$$

The photoluminescence (PL) energy is given as[6]

$$E_{PL} = E_G - W \tag{9}$$

where  $W$  is thermalization energy, from equation (2) and equation (3),  $W$  is given by [9]

$$W = Aq_0^2 \tag{10}$$

$$E_c(q) - E_v(q) = \hbar\omega = E_G + \frac{\hbar^2 q^2}{2\mu} \tag{11}$$

where  $\mu$  is the reduced mass for the e-h pair, this equation is for free electron model, but for confinement electron the subbands is quantization, each has a bottom energy of (with estimate to the band edges) [13]

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2m^* L_x^2} \quad (12)$$

where  $n$  is a quantum number (is an integer),  $L_x$  width of quantum well and  $m^*$  is the effective mass, for amorphous silicon it equal  $0.24m_o$  [14].

For quantum dot in three dimensions [18]

$$E_{n,m,k} = \frac{\hbar^2 \pi^2}{2m^*} \left( \frac{n^2}{L_x^2} + \frac{m^2}{L_y^2} + \frac{k^2}{L_z^2} \right) \quad (13)$$

The equation (11) become

$$E_c(q) - E_v(q) = \hbar\omega = E_G + \left[ \frac{\hbar^2 \pi^2}{2m^*} \left( \frac{n^2}{L_x^2} + \frac{m^2}{L_y^2} + \frac{k^2}{L_z^2} \right) \right] \quad (14)$$

Where assuming that the energies levels in the three dimensions are non-degenerate, i.e,  $n = m = k$  and  $L_x = L_y = L_z = R$

$$E_c(q) - E_v(q) = \hbar\omega = E_G + \left[ \frac{3n^2 \hbar^2 \pi^2}{2m^*} \left( \frac{1}{R^2} \right) \right] \quad (15)$$

As it was assumed,  $\frac{1}{R^2} = q^2$

$$E_c(q) - E_v(q) = \hbar\omega = E_G + \frac{3n^2 \hbar^2 \pi^2 q^2}{2m^*} \quad (16)$$

By making equation (2) equal to equation (14)

$$E_G + 2Aqq_0 - Aq_0^2 = E_G + \frac{3n^2 \hbar^2 \pi^2 q^2}{2m^*}$$

$$\frac{3n^2 \hbar^2 \pi^2 q^2}{2m^*} = A(2qq_0 - q_0^2)$$

$$A = \frac{\frac{3n^2 \hbar^2 \pi^2 q^2}{2m^*}}{(2qq_0 - q_0^2)} \quad (17)$$

From equation (14) we can be obtain expression of  $q$  as

$$q^2 = \frac{(\hbar\omega - E_G)2m^*}{3n^2 \hbar^2 \pi^2}$$

$$q = \sqrt{\frac{(\hbar\omega - E_G)2m^*}{3n^2 \hbar^2 \pi^2}} \quad (18)$$

$$\therefore q_0 \propto d_i^{-1} \quad (19)$$

$$q_0 = \frac{C_i}{d_i} \quad (20)$$

$$C_i = \frac{d_i}{d_0}$$

$$\therefore q_0 = \frac{1}{d_0} \quad (21)$$

The real component for dielectric constant  $\epsilon_r(\omega)$  refers to the polarization aspects of the electronic system. Although the real part  $\epsilon_r(\omega)$  and imaginary part  $\epsilon_r'(\omega)$  of the complex dielectric function describe physically distinct phenomena, they are in fact mathematically related by an important theorem known as the Kramers-Kronig relation, may be written as [15]:

$$\epsilon_r(\infty) - 1 = \chi = \frac{2}{\pi} \int_{\omega_0}^{\infty} \frac{\epsilon_r'(\omega)}{\omega} d\omega \quad \text{where} \left( \omega_0 = \frac{E_{PL}}{\hbar} \right) \quad (22)$$

When substituting equation (8) in equation (22) we get

$$\epsilon_r(\infty) - 1 = \chi = \frac{Ff_{cv}}{A^2q_0} \int_{\omega_0}^{\infty} \frac{\hbar\omega - E_{PL}}{\omega^3} d\omega \quad (23)$$

$$= \frac{\hbar^2 Ff_{cv}}{2A^2q_0E_{PL}} \quad (24)$$

Where  $\hbar\omega - E_{PL} = 2Aqq_0$  as specified by equation (3). therefore, the size reduced dielectric susceptibility relies in practice on the features of electron-phonon coupling and the photoluminescence energy.

### 3. RESULTS AND DISCUSSION

As it was mentioned earlier the miniaturizing of a semiconductor tendency the expansion of band gap (EG) [6] due to the inner core level to shift towards higher binding energy [16]. When taking the sizes of quantum dots from (1.8 nm to 12 nm), we found that the energies gaps corresponding of these sizes are (4.523 eV to 1.627 eV) taking in account that the value increasing is 0.6 nm, and depending the relation that describe the energy gap,  $E_{QD}$ , for a three dimensionally confined amorphous silicon quantum dots(a-SiQDs) model as give [17-19]:

$$E_{QD} = E_{g(bulk)} + \frac{C}{\left(\frac{D}{2}\right)^2} \quad (25)$$

where  $E_{g(bulk)}$  is the band gap for bulk amorphous silicon which estimate (1.56 eV) that have been deduced through data of empirical scales. The values referred to in literature for bulk a-Si which is (1.5 -1.6) eV [20] are very coincide with this value. Where,  $C$  is the parameter for confinement that is limited likely (2.4 eV nm<sup>2</sup>) and  $D$  is the diameter of the dot. As shown in figure (2).

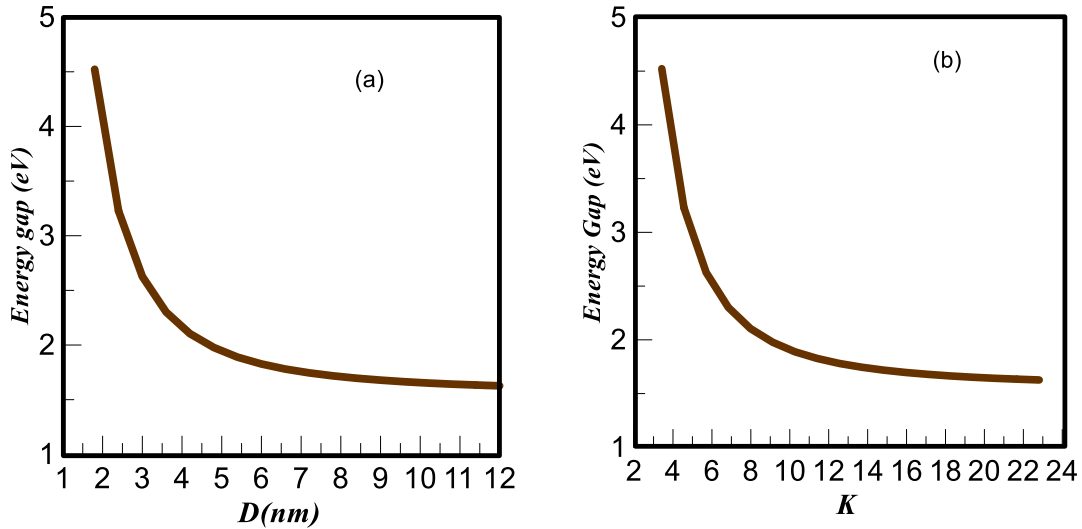


FIGURE (2): Effect of the confinements on the energy

gap as a function of: (a) the quantum dot size  $D$  (nm), and (b) with  $(K=D/2d)$  the number of atoms that alignment in radius of nanodot.

In this work the sizes of quantum dots of amorphous silicon were selected in the range of 1.8 nm to 12 nm, depending on the equation (25), so as to obtain an approximately equal value of the energy gap of about equal 1.6 eV, which is the value of the energy gap of amorphous silicon in the case of the bulk.

It was noted that for each size of quantum dots its own range of energy (frequency) and it is embodied in the equation (16) where the energy gap varies with the size of the dot, and accordingly the wave vector values is change. We note that the smaller quantum dot size which was used in this work, (1.8 nm) requires a larger extent of energy, which starts from 5.536 eV to 9.036 eV then the energy gradually decreased with greater quantum dot size. It was found that when the quantum dot size reach to 12 nm find that the extent of energy becomes from 2.963 eV to 3.243 eV. Since we have attempted in this work to decrease the value of the dielectric constant to about 11.7, which is the value of bulk in amorphous silicon to the lowest possible value obtained using the an appropriate energy or the frequency for that size of amorphous silicon. We have observed that the value of dielectric constant of amorphous silicon of quantum dots reach to the lowest value which is equal to 1.199 for dot size 1.8 nm, which corresponds to the largest value of energy or frequency of that size. The study also shows that the dielectric constant values begin to increase gradually with increasing the quantum dot size of amorphous silicon up to 7.595, which is the dielectric constant value for dot size 12 nm as shown in figure (3). We note that the range of the energy which used extends from the violet in the visible region even the extreme in the ultraviolet region (on the electromagnetic spectrum).

Reduction of quantum dot size leads to the increase of crystal binding energy which represents band gap (EG) that require increasing of photo absorption to electron transition from the lower valence band to the excited state in conduction band, as well as electron-phonon interaction become more important due to nanometric system, where e-p interaction contributes in to the transmission of electron, resulting decrease in the dielectric constant. Note that there are different values of the dielectric constant for each size corresponding to the energy or frequency values but we relied on the interview of the largest energy values (frequency) as we have said previously to obtain at the highest intensity of photosensitivity of different sizes mentioned. At low frequency, the dielectric loss has high values, then it at higher frequencies begin to reduce. The dispersion at low frequency in the dielectric loss is attributed to charge carriers that results to high missing at low frequencies.

It's possible singles the deferent polarization components through gauging the dielectric constant as a function to frequencies. Where there are a restricting featured frequency for each polarization mechanism. Because a very small mass for the electrons, as a result can be relay large frequencies during the optical extend. Ions are relay fields up to IR range due to their weight which are heavier from the electrons by thousand times. Molecules are heavier so far and are strongly obstruction by their surroundings. Although the interfacial are mostly in the kilohertz range or less frequency but it's owning an significant influence on the polarization process of a dielectric constant. The

contribution of the polarization mechanism can be desert when the applied field has frequency is completely higher with comparison to the adverse of the relaxation time for that polarization process.

The mechanics of polarization relies on the movement of particles with mass. Particles should be accelerated and shifted back and forth as the electric field changes, which cannot ensue promptly. As some movements of particles involve the movement of different masses and different distances, the different types of polarization will have different rates at which polarization occurs. When a time varying electric field is applied, dielectric constant depends on the frequency for field. All types for polarization possess time to reach their relaxed state at low frequencies, with the increase of frequency, the slower processes do not have time to totally relax in advance to the changes of polarity of the electric field. Consequently, the slower processes cease to contribute to the dielectric constant [21]. Conversely, at high frequencies the dielectric loss is mainly because of dipole rotations or of ionic transitions from the lower energy states to higher energy states. Due to the upward transition, the energy is absorbed from the applied field. The absorption of energy is possible if orientational polarization or permanent dipole moments are present [22].

The larger value of dielectric constant at lower frequencies is owing to the all contribution (atomic, electronic, ionic and interfacial polarization). With the increase of frequency, the contribution from the space charge (interfacial) and orientational polarization reduces so dielectric constant decreases. The dielectric constant completely ceases at higher frequency [22].It should be noted by figure(3), it can be divided these volumes into two regions: the first region includes the dot size which has the range between  $(1.8 \leq D < 6.4 \text{ nm})$  and take the form of an almost straight line to the values of dielectric constant this means that the quantum confinement clearly shows in this region of work. The second region is that the dot size taken within the range  $(D \geq 6.4 \text{ nm})$  it's bulk-like behavior, where we find that the straight line begins to bend at Size 6.4 nm, where takes the form of saturation almost this means that the quantum confinement become weak in this range of quantum dots size, although the size of the semiconductor still the nanoscale. On this basis, we can say that the sizes of quantum dot from 1.8 to 6.4 nm would be suitable for this work.

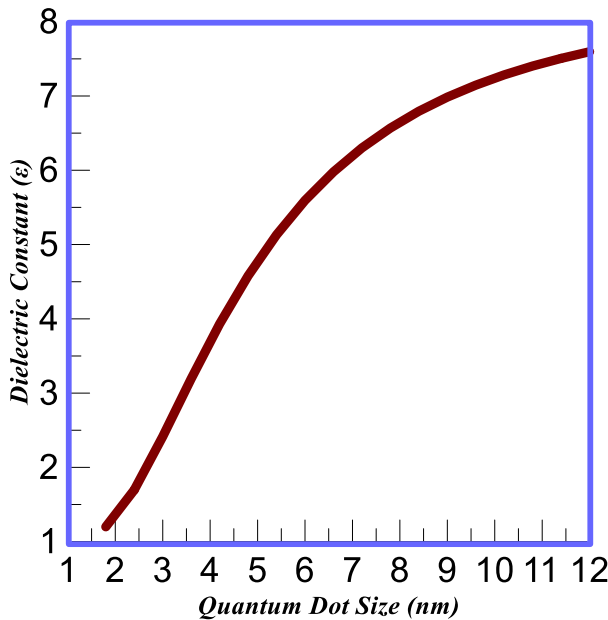


FIGURE (3): The dielectric constant of a-SiQDs versus quantum dot size.

CONCLUSIONS

In summary, for the nanosolid some the particular solicitude of optical and electronic properties i.e., the expansion of band gaps which reason the blue shift in photoluminescence, the inner energy level of the core band to shift simultaneously towards higher binding energy and the dielectric constant is reduced and reason a blue shift in photo absorption. The complex dielectric constant is related to the band gaps which is specified by the crystal filed. Decreasing of the quantum dot size resulting to the reducing of the dielectric constant because the increasing in the

band gap and electron-phonon interaction. As well as, energy incident dependence of the reduction of the dielectric constant due to decreases in the process of polarization.

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