Studies Of Silicon Quantum Dots Thin Films Deposited Under Disparate Ambient Argon Pressures

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Abstract- This research presents the synthesis, optical and electrical studies of Si quantum dots prepared by Physical Vapour Condensation Technique at the working pressure of 15 Torr and 20 Torr. The synthesized quantum dots were characterized by FESEM, X-ray diffraction and UV/VIS/NIR spectroscopy. The X-ray diffraction pattern of synthesized quantum dots shows the amorphous nature. FESEM images suggest that the size of quantum dots varies from 6-8 nm. On the basis of UV-visible spectroscopy measurements, a direct band gap has been observed. The temperature dependence of dc conductivity of Si quantum dots films have also been studied in the temperature range 300 to 450. It is evident that the dc conductivity (σ_{dc}) increases exponentially with increasing temperature, indicating that conduction in these quantum dots is through an activated process which also shows the semiconducting performance of synthesized quantum dots.

Index Terms- Si Quantum Dots, Thin Films, XRD, Optical Properties, Electrical Properties

I. INTRODUCTION

Silicon is a semiconductor of unparalleled technological versatility, and its nanoparticle form has attracted a great deal of interest for a broad variety of applications. Silicon nanoparticles exhibit quantum confinement, making them useful for optoelectronic devices and photo catalysis; however, the optoelectronic properties of a given particle are known to depend in poorly understood ways on the particle size, shape, and surface termination. For medical applications, silicon's apparent nontoxicity [1] and fluorescent properties make it an attractive base for nanoparticle-based diagnostics and therapeutics. Silicon is also attractive as an anode material for Lithium ion batteries due to its low discharge potential and extremely high theoretical charge capacity [2]; however, the tendency for silicon to expand dramatically as it absorbs Lithium means that anode morphology must be carefully controlled to avoid breakage [3]. For applications in photovoltaic, nanostructured silicon has attractive properties including relatively low cost, low toxicity, and the possibility of multiple exciton generation [4]. For many applications, an increased level of control over nanoparticle shape and the exposure of different surface facets are strongly desirable; shape-engineered nanoparticles may allow detailed control of optical properties while selective functionalization of different surfaces may allow catalytic and self-assembling properties of nanoparticles to be exploited.

The quantum dots (QDs) offer the impressive ability to harvest sunlight, advantageous features of photo stability, high molar extinction coefficients, size dependent optical properties and low costs. In the near future, the single-electron Nano devices and molecular devices will be manufactured as higher integrated circuits [5]. The optical interconnects are expected for the higher integrated circuits and three-dimensional circuits. Many types of optical interconnect have been developed and discussed: optical interconnects between circuit boards in the computer, between chips, and between individual elements within in a chip [6]. The study towards a full understanding of synthesis and properties of Si nanoparticles is still under way [7]. Now a days, a lot of research work is going on to investigate the Si quantum dots for solar cell applications. Kintz et al. [8] has synthesized Si quantum dots/ SiO_2 composite films for its application in third generation solar cells. Waheed A. Badawy [9] has made a review on solar cells from Si quantum dots. Yu et al. [10] has studied the effect of phosphorus incorporation on electrical and optical properties of Si quantum dots/SiO_2 films. Li et al. [11] has studied the enhanced photo electrochemical water splitting from Si quantum dots. Shi et al. [12] has studied the improvement of Graphene-Si solar cell. Guha et al. [13] has studied

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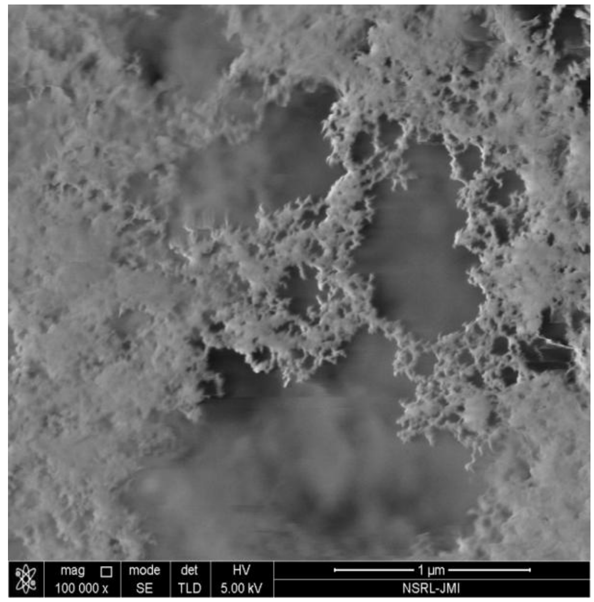
the amorphous and Nano crystalline Si solar cell and its module. Hung et al. [14] has studied the enhancement of efficiency of Si Solar cell through a downshifting and antireflective oxysulfide phosphor layer. Xu et al. [15] has studied the spectral characteristics of carrier transfer from Si cluster to Nano crystal in Si rich Oxide/SiO_2 multilayer films. Schimmoeller et al. [16] has studied the synthesis of Si and tin doped Si powder for Li –ion batteries. Shah et al. [17] has made a review on preparation of Si nanomaterials by arc discharge. The present research work describes the Synthesis and characterization of Si quantum dots prepared at various working pressure.

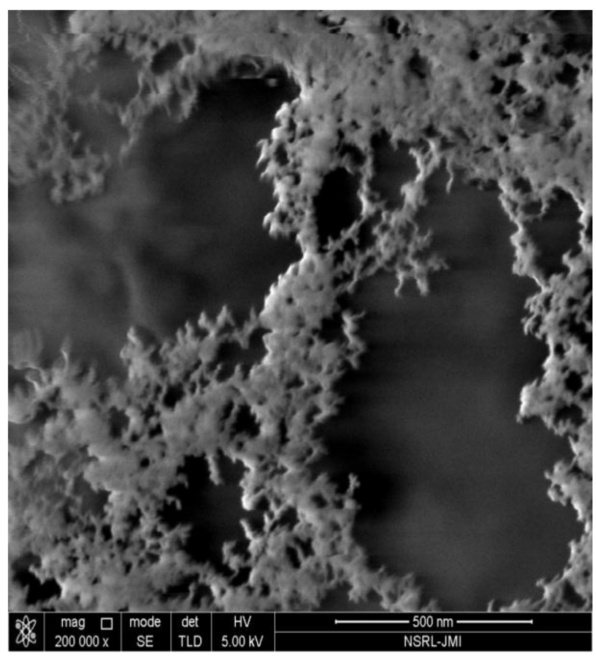
II. EXPERIMENTAL

Si quantum dots were synthesized by Physical Vapor Condensation Technique. A small piece of Si was placed in a graphite boat in a vacuum chamber. The chamber was evacuated to 10^{-6} Torr using molecular turbo pump. The chamber was purged with argon gas at two different pressures (15 and 20 Torr) and then, the quantum dots were grown directly on silicon wafer substrate cooled by liquid nitrogen. The quantum dots of different sizes were obtained under argon pressure of 15 and 20 Torr. The surface morphology of these quantum dots was determined by Field Emission Scanning Electron Microscope (FESEM) while the amorphous nature was confirmed by X-ray diffraction studies. The absorption of the prepared Si quantum dots were studied by JASCO UV/VIS/NIR spectrophotometer. For dc conductivity measurements, silver paste was used as thick electrode on the thin films. The prepared thin films were then mounted in a specially designed metallic sample holder, where a vacuum of about 10^{-2} Torr was maintained throughout the measurements. A dc voltage was applied across the sample and the resulting current was measured by a digital electrometer (Keithley, Model-617). The temperature of the film was increased from 300 to 450 K by a step value of 5 K and correspondingly the current was read by the electrometer.

III. RESULTS AND DISCUSSIONS

The morphology of silicon quantum dots prepared at 15 Torr and 20 Torr working pressure has been investigated using Field Emission Scanning Electron Microscope (FESEM-Nova Nano Sem450, FEI) which is shown in Fig. 1. It is observed that the prepared films contain quantum dots of average size of about 6-8 nm.





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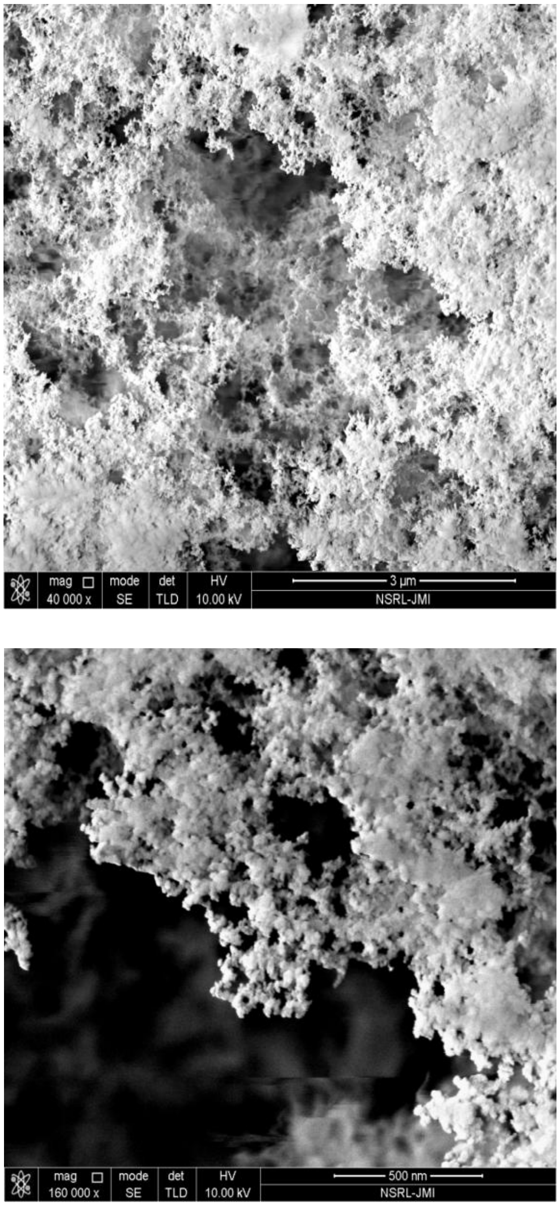

Fig. 1: FESEM images of Si quantum dots at different magnification prepared at (a-b) 15 Torr and (c-d) 20 Torr working pressure.

The X-ray diffraction of quantum dots thin films have been recorded by using a Rigaku Ultima IV diffractometer [copper target was used as the source with λ = 1.54056A° (Cukα1)]. The range of scanning is set from 10° – 80^0 at the rate of 2^0/min. The XRD patterns are shown in the Fig. 2. We have not observed any significant peak in XRD pattern, which suggest the amorphous nature of synthesized quantum dots.

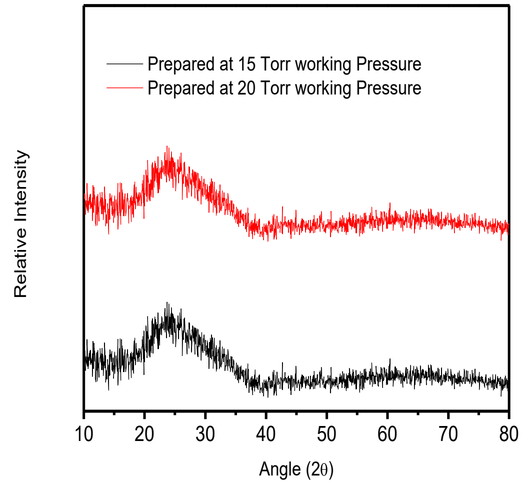

Fig. 2: X-ray pattern of Si Quantum Dots thin films prepared at 15 Torr and 20 Torr argon pressure.

The optical properties of Si quantum dots have been studied at room temperature and a wavelength range of 300-900 nm was chosen for recording the optical absorption. The optical density recorded using UV/VIS/NIR spectrophotometer can be converted into absorption coefficient (α) using the following relation [18-19].

α = Optical Density/ Film Thickness --------- (1)

The absorption coefficient has been calculated by using above relation and is shown in Fig. 3. It is found to be increases exponentially with the increase in photon energy for the both the samples. The quantum dots fabricated at higher argon gas pressure (20 Torr) show higher absorption as compared to that of prepared at lower chamber pressure (15 Torr). This is due to size effect.

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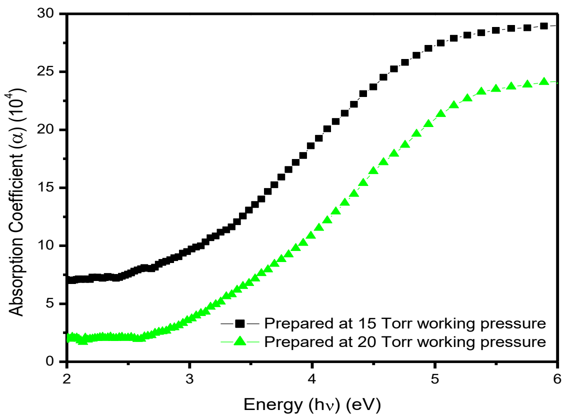

Fig. 3: Absorption coefficient (α) against photon energy (hν) for Si Quantum dots thin films

To calculate the optical band gap of a material, we use the following relation [20-24]

$(\alpha h\nu)^{1/n} = B\,(h\nu - E_g)$ ---------- (2)

where, ν is the frequency of the incident beam, B is a constant, E_g is the optical band gap and n is an exponent. The values of n can be taken as 1/2, 3/2, 2 and 3 for different electronic transitions responsible for absorption [21-23]. The present system of silicon quantum dots follows the rule of direct transition. On the basis of direct transition, Equation (2) is rewritten as given below:

$(\alpha h\nu)^2 \propto (h\nu - Eg)$ ------------ (3)

The dependence of $(\alpha h\nu)^2$ with photon energy (hν) for as-deposied silicon quantum dots is shown in Fig. 4.

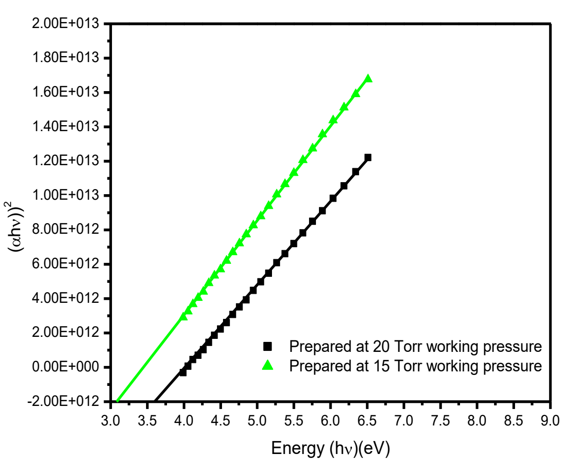

Fig. 4: $(\alpha\, h\nu)^2$ versus photon energy hν (eV) for Si quantum dots thin films

The values of energy gap have been calculated by taking the X-axis intercepts of Fig. 4. The calculated values of E_g are listed Table 1. The increase in the value of optical band gap with the increase in ambient gas pressure in the chamber is due the reduction in the size of quantum dots which is also confirmed the FESEM.

The electrical transport property of the materials is an important factor which reveals the significant and reliable information about the transport phenomenon and other physical properties of the material.

The dc conductivity can be expressed by the relation,

$\sigma_{dc} = \sigma_0 \exp(-\Delta E_c / KT)$ ------- (4)

or

$\ln \sigma_{dc} = -(\Delta E_c / 1000\,K)(1000/T) + \ln \sigma_0$ ------(5)

where, σ_0 and ΔE_c represents the pre-exponential factor and activation energy respectively, K is the Boltzmann constant.

When we plot a graph between ln σ_{dc} and 1000/T, a straight line is obtained having slope $(\Delta E_c / 1000\,K)$.

We may calculate the activation energy (ΔE_c) as follows,

$(\Delta E_c) = 1000\,K \times$ slope of straight line ------- (6)

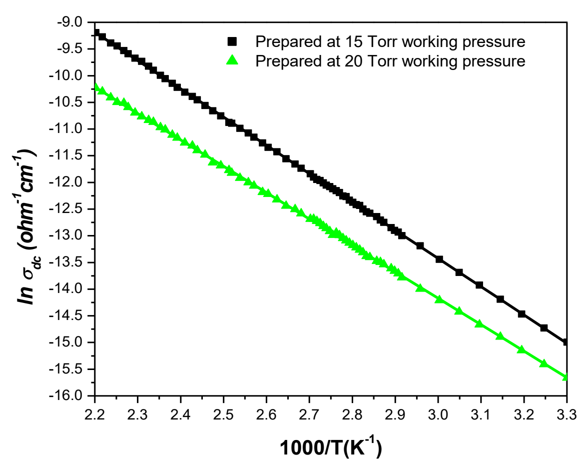

Fig. 5: Temperature dependence of dc conductivity in the temperature range (300 to 450 K) of Si Quantum dots thin films

The temperature dependence of the dc conductivity of thin films of Si quantum dots prepared at 15 Torr and 20 Torr working pressure in the temperature range 300 to 450 K have been studied and are shown in Fig. 5. It is evident from this figure that the dc conductivity (σ_{dc}) increases exponentially with increasing temperature, indicating that conduction in these quantum dots is through an activated process, which also shows the semiconducting behavior of these quantum dots. The variation of dc conductivity with different working pressure is shown in Table 1.

Table-1
Optical and electrical constants in Si Quantum Dots prepared at different ambient argon pressures

Ambient Argon Pressure	Absorption Coefficient (cm^{-1}) At λ= 450 nm	Optical Band Gap (eV)	σ_{dc} ($\Omega^{-1}cm^{-1}$) At T= 375 K	ΔE_{c} (eV)
15 Torr	456 x 10^4	3.11	2.83 x 10^{-5}	0.52
20 Torr	495 x 10^4	3..62	3.64 x 10^{-5}	0.65

The calculated values of activation energy are given in Table 1. It is evident from this table that the conduction is due to thermally assisted tunneling of charge carriers in the localized states of band tails. The dc conductivity increases by orders of magnitudes as the working pressure increases. An increase in dc conductivity with a corresponding increase in activation energy is found to be associated with shift of the Fermi level [25-26]. However, it has also been pointed out that the increase in conductivity could be caused by the increase in the portion of hopping conduction through defect states [27].

IV. CONCLUSION

This research work focuses on the structural, optical and electrical properties of Si quantum dots prepared by physical vapor condensation technique at 15 Torr and 20 Torr working pressures. FESEM investigations suggest the formation of silicon quantum dots of average size 6-8 nm. HRXRD studies reveal the amorphous nature of synthesized quantum dots. An increased optical band gap with increasing working pressure is observed, which is due to the formation of very small size quantum dots. This may also be due to the formation a large number of energy tails extending beyond the band gap. This high energy contribution is due to the electron hole recombination. The dc conductivity (σ_{dc}) increases exponentially with increasing temperature, indicating that conduction in these quantum dots is through an activated process which also shows the semiconducting behavior of these alloys. An increase in dc conductivity with a corresponding change in activation energy is found to be associated with shift of the Fermi level.

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