

STUDY OF THE EFFECT OF NANOPARTICLE SIZE ON THE DIELECTRIC CONSTANT AND CONCENTRATION OF CHARGE CARRIERS OF Si AND CdS MATERIALS

H. A. ABID*, S. N. T. AL-RASHID

Department of Physics, College of Education for Pure Science, University of Anbar, Iraq

In this research, the effect of nanoparticle size on the dielectric constant and the concentration of charge carriers in silicon (Si) material and cadmium sulfide (CdS) is studied. These properties are studied by using a computer program in MATLAB version (17). This program depends on the Brus model and the characteristic matrix theory. The results indicate that the dielectric constant increases with the increase in the granular size of the material and when the granular size decreases the dielectric constant decreases. As for the concentration of the charge carriers, we notice that it decreases with the decrease of the granular size of the material.

(Received September 27, 2020; Accepted December 12, 2020)

Keywords: Concentration of charge carriers, Dielectric constant, Bruce model, Characteristic matrix

1. Introduction

The study of the electrical properties of semiconductor nanoscale materials is of great importance, as they are included in many important industrial applications, especially in the manufacture of energy devices and optical sensors. Semiconductors with nanostructures have a unique variety of optical, electrical and electronic properties that are different from the properties that are available in Bulk Materials [1]. The most important distinguish semiconductor nanoparticles is the increase in the surface area relative to the size of the nanomaterial, addition to that the energy gap, is wide range as it plays an important role in the electrical and optical properties of semiconductor materials, and this change in properties appears mainly due to the quantization of energy levels of electrons. Within a specific size, this is known as quantum confinement [2]. When the crystal size decreases to become close to or smaller than the de Broglie wavelength, the distance between energy levels increases, so the quantum confinement affects the energy gap and the density of material states, and thus the electrical and electronic properties. Thus, these properties depend on the sizes of the nanoparticles also known in the case as quantum dots, in which the movement of electrons and holes is restricted in all three directions [4, 3].

2. The theory

2.1. Effective mass approximation (EMA) model

It is one of the important theoretical models that shows how the energy gap in the quantum dots in semiconductors depends on the size of the particle, and it is often called the Brus model. The value of the change in the energy gap in the quantum points (ΔE_g) is given the Brus equation [5]:

$$\Delta E_g = \frac{\hbar^2 \pi^2}{2R^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right] - \frac{1.786 e^2}{\epsilon R} - \frac{0.124 e^4}{h^2 \epsilon^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right]^{-1} \quad (1)$$

* Corresponding author: ahiba078@uoanbar.edu.iq

R represents the radius of the particle as a spherical quantum point

m_e^* Effective mass of the electron

m_h^* the effective mass of the hole

ϵ Relative permittivity, or what is known as the dielectric constant.

Since $\Delta E_g = E_g^{nano}(R) - E_g^{bulk}$ equation (1) takes the form [6]:

$$E_g^{nano}(R) = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2R^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right] - \frac{1.786 e^2}{\epsilon R} - \frac{0.124 e^4}{\hbar^2 \epsilon^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right]^{-1} \quad (2)$$

From the second term on the right-hand side of equation (2), we notice that the energy gap is inversely proportional to R^2 , meaning that the energy gap decreases when the nano particle size increases. The third term in the equation can be neglected due to the increase in the strength of the columbic interaction, where it led to a decrease in the energy gap with decreasing R . The smallness of the third term and last term compared to the second term allows it to be neglected. So equation (2) becomes

$$E_g^{nano}(R) = E_g^{bulk} + \frac{\hbar^2 \pi^2}{2R^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right] \quad (3)$$

As a result of quantum confinement, we notice that the energy gap increases with decreasing nano-particle size. Whereas, the quantum confinement is large when the particle radius of the substance becomes smaller or equal to the natural Bohr radius α_0 of the exciton

$$\alpha_0 = \frac{4\pi\epsilon_0\epsilon_r\hbar^2}{e^2} \left[\frac{1}{m_e^*} + \frac{1}{m_h^*} \right] \quad (4)$$

If ϵ_r and ϵ_0 present the dielectric constant of the vacuum and the semiconductor material, respectively, and e represents the electron charge.

2.2. Refractive index

The optical properties of a semiconductor material can be determined by its refractive index according to the following relationship:

$$n = c / v \quad (5)$$

where c represents the speed of light in vacuum ($3 \times 10^8 \frac{m}{sec}$), while v is the speed of light in the medium.

In semiconductor materials, the refractive index is closely related to the energy E_g , and the value of the refractive index of the material changes with the change of the wavelength of the incident light, but this change is very small as it results from the change in the velocity of the waves in the material as a result of the interaction difference of the material with the rays and according to their frequency, as well as the value of the refractive index affected by the change in temperature, but this change is very weak [8, 9]

There have been many attempts to find mathematical formulas linking the refractive index with the energy gap, as in the following relationship:

$$n = \alpha + \beta E_g \quad (6)$$

As: ($\alpha = 4.048$) and ($\beta = -0.62 \text{ eV}^{-1}$) This equation is independent of the temperature, and we notice that the value of the refractive index decreases with the increase of the energy gap.

2.3. The characteristic matrix

When an electromagnetic radiation falls on a surface separating two media of different optical properties, the value of the reflectivity for the incident ray is given by Fresnel's equations: [10]

$$R = \left(\frac{\eta^\circ - \eta_1}{\eta^\circ + \eta_1} \right)^2 \quad (7)$$

where η_1 and η° represent the optical permittivity or the effective refractive index for the incidence and penetration modes, respectively.

The value of the optical permittivity of the medium in for the vertical incidence of the wave is equal to the real part of the refractive index [11]:

$$\eta = y = n \vartheta = n \quad (8)$$

where n is the real part of the refractive index of the medium, and ϑ is the admittance of free space. Its value may be neglected because it is very small ($2.65 \times 10^{-3} S$)

In the case of an oblique incidence, the optical permittivity of the single medium is separated into two parts, namely the optical permittivity of parallel polarization (η_p) and the optical permittivity of the vertical polarization (η_s) due to the phenomenon of polarization and is given by the following formulas [10]:

$$\eta_{\circ p} = n_{\circ} / \cos \theta_{\circ} \quad (9)$$

$$\eta_{1p} = n_1 / \cos \theta_1 \quad (10)$$

$$\eta_{\circ s} = n_{\circ} \cos \theta_{\circ} \quad (11)$$

$$\eta_{1s} = n_1 \cos \theta_1 \quad (12)$$

where: η_{1p} and $\eta_{\circ p}$ represent the optical permittivity of the incidence and penetrating medium respectively in the case of the plane polarization P,

(P, η_{1s} , $\eta_{\circ s}$) represent the optical permittivity of the incidence and penetrating medium respectively in the case of vertical polarization (S), θ_{\circ} represents the angle of incidence.

And when the electromagnetic radiation incidence on a single thin film consisting of two separating limits and deposited on substrate material as in Fig. 1:

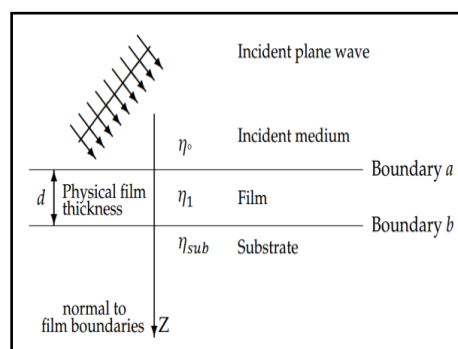


Fig. 1. Incident plane wave on a thin film [12].

In the case of the vertical and oblique incidence, and for any of the polarizations, the optical permittivity of the system can be determined through the characteristic matrix [13], which links the continuous tangential components of the electric and magnetic fields falling on and out of the system, and it is given as the following formula [14].

$$\begin{bmatrix} B \\ C \end{bmatrix} = \begin{bmatrix} \cos\delta & i\sin\delta/\eta_1 \\ i\eta_1\sin\delta & \cos\delta \end{bmatrix} \begin{bmatrix} 1 \\ \eta_{sub} \end{bmatrix} \quad (13)$$

(B, C) represent the elements of the matrix, which represent the electric and magnetic field η_1 represents the optical permittivity of the membrane, η_{sub} represents the optical permittivity of the substrate, while delta represents the phase thickness, which is given by the following relationship:

$$\delta = 2\pi n_1 d_1 \cos\theta_1 / \lambda$$

And here is all the information required to find the value of the optical permittivity entering a system consisting of a single thin film deposited on the surface of a substrate. It is provided through equation (13), and thus the value of the reflectivity of the system can be found through equation (7).

3. Applications

In this study, a computer program was designed in (MATLAB) version (17) to study the values of the dielectric constant and concentration of charge carriers) as a function of the change of the nano particle size for Si, and CdS.

3.1. Dielectric constant of (Si, CdS)

Here, we study the change in the dielectric constant value of silicon Si and cadmium sulfide CdS as a function of the nanoparticle size. Figs. 1 and 2 show the change in the dielectric constant values of the materials as a function of the change of the nanoparticle size:

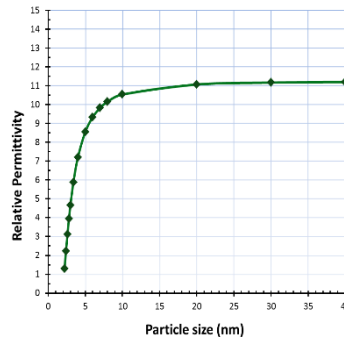


Fig. 1. Change of the dielectric constant of silicon (Si) as a function of change in the nanoparticle size.

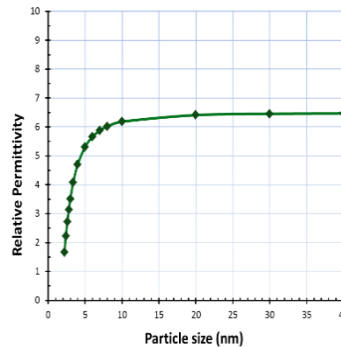


Fig. 2. The change in the dielectric constant of cadmium sulfide (CdS) as a function of change in the nanoparticle size.

From observing the shapes, we find that the dielectric constant increases with the increasing size of the material. To explain this, we can use the fact that in the nanoscale, the ratio of the surface area compared to the volume is very large, and this means that the number of atoms on the surface compared to the size is very large. In the nano scale range, the electron orbits contracts that causes increment in the coulombs force, which enhances restoring force, that is, the natural angular frequency of the electron oscillation increases, causing the dielectric constant decrease. This proves that the dielectric constant decreases with the particle size of the material [15]. The above results are consistent with previous research.

Z. Cai (2018) found that as grain size decreases, the particle size ratio increases, as mentioned above. The dielectric permittivity within the boundaries of the granules is much less than that of the granules. Consequently, the effective permittivity of the dielectric will decrease as the grains of silicon (Si) nanomaterials (Si) and cadmium sulfide (CdS) become smaller [16].

3.2 Concentration of charge carriers for Si and CdS

The following figures (3) and (4) illustrate the study of the change in the concentration of charge carriers of Si and CdS with the change of the particle size of the material:

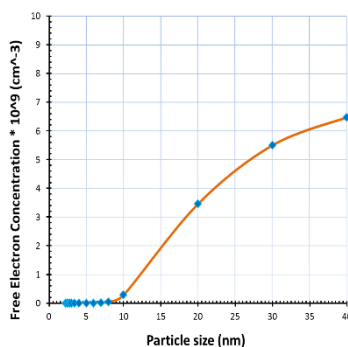


Fig. 3. The change in the concentration of charge carriers for the silicon (Si) as a function of the change in the nanoparticle size.

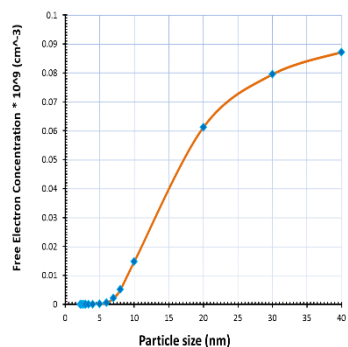


Fig. 4. The change in the concentration of charge carriers of cadmium sulfide (CdS) as a function of change in the nanoparticle size.

We observe the change of the charge carriers of the studied materials as a function of nanoparticle size, we notice when the size of the object is very small, the concentration of the charge carriers is very small and this is definitely due to the quantitative reservation of the electron for the small sizes, as the atoms present on the surface are few and the atomic groupings are around 10 to 50 atoms. As for when the nanoscale size increases, the concentration of charge carriers increases dramatically and this is expected as the greater the size of the granular body, the greater the number of atoms and molecules on the surface. In other words, the increase in the

charge carriers (electrons and holes) in the semiconductors and thus the conductivity of the materials increases according to the increase of these carriers and this behavior has been done. It was noted by P. Parameshwari (2012) that the increase in electrical conductivity can be attributed to the decrease in dispersion that occurs at the grain boundaries when the grain size increases and the crystallinity improves, which leads to increased mobility and injection of free charge carriers [17].

4. Conclusions

Most semiconducting materials behave similarly to when the material size decreases from its normal size (Bulk Size) due to volume quantization. This behavior arises because the size of the nanoparticles is comparable to the de Broglie wavelength of their charge carriers (i.e. electrons and holes). We notice that the energy gap value is large at small volumes and then gradually decreases when increasing the size of the object until it becomes almost constant after the granular size of the material exceeds the bor radius of the exciton for most materials, and that an increase in the value of the energy gap at small volumes leads to a change in the electrical properties of the material.

The study of the electrical properties of these materials is very important as they are used in many applications of optoelectronics. One of its most well-known applications is the fabrication of dual-link lasers, CD-reading, as well as manufacturing many LED lights. Among the most important electrical properties (dielectric constant and concentration of charge carriers), and the results in this study indicate that the dielectric constant of the two materials (Si and CdS) increases with the increase in the size of the material and decreases with the decreasing size, as well as for the concentration of the charge carriers for materials (Si and CdS), we notice that it decreases as the granular size decreases and increases with the granular size of the substance.

References

- [1] Ulrike Woggon, *Optical Properties of Semiconductor Quantum Dots*, Springer-Verlag Berlin Heidelberg, Germany, (1997).
- [2] A. Scaff, *Introduction to Nanotechnology (Science, Engineering & Applications)*, Series of Strategic and Advanced Techniques, Arabic Compendium of Translation, (2011), INSB: 139789953824437.
- [3] A. Scaff, *Introduction to Nanotechnology, (Science, Engineering & Applications)*, Series of Strategic and Advanced Techniques, Arabic Compendium of Translation, (2011), NSB: 139789953824437.
- [4] Guozhong Cao, *Nanostructures and Nanomaterials: Synthesis, Properties, and Applications*, Imperial College Press, (2004).
- [5] Shashank Sharma, Ravi Sharma, *International Scientific Journal* **2**(1), 120 (2015).
- [6] Z. L. Wang, Yi Liu, Ze Zhang, *Handbook of nanophase and nanostructured materials II*, Kluwer Academic Plenum, (2003).
- [7] B. Bhattacharjee, D. Ganguli, K. Iakoubovskii, A. Stesmans, S. Chaudhuri, *Indian Academy of Sciences* **25**(3), 175 (2002).
- [8] C. Z. Tan, J. Arndt, *Journal of Physics and Chemistry of Solids*, 1315 (2000).
- [9] Bradley J. Frey, Douglas B. Leviton, Timothy J. Madison, *SPIE-The International Society for Optical Engineering*, (2006).
- [10] Michael Bass, *Handbook of Optics: Fundamentals, techniques, and design*, Second Edition, McGraw-Hill Education, 1995.
- [11] J. J. Zhong, A. R. L. Travis, F. P. Payne, J. R. Moore, *The Antireflection Coating for a Wedge Flat Panel Projection Display*, Convention Centre, San Jose, California, 914 (2001).
- [12] Yusuf Simsek, *Development of Software for Calculations of The Reflectance, Transmittance and Absorptance of Multilayered Thin Films*” M.Sc. Thesis, Middle East Technical University, Turkey, 2008.
- [13] Alaa J. Ghazai *J.Thi-Qar Sci.* **1**(2), 79 (2008).

- [14] H. Angus Macleod, *Thin-Film Optical Filters*, Fourth Edition, CRC Press, Taylor & Francis Group, LLC, 2010.
- [15] W. H. Qi., *Physica B* **368**, 46 (2005).
- [16] Z. Cai, X. Wang, W. Hong, B. Luo, Q. Zhao, L. Li, *Journal of the American Ceramic*, 2018.
- [17] P. Parameshwari, B. Shashidhara, K. Gopalakrishna, *Arch. of Physics Research* **3**, 441 (2012).