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# Shape Dependent Optical Properties of GaAs Quantum Dot: A Simulation Study

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The present paper deals with the simulation study of the GaAs quantum dot with different shapes such as cuboid, cylinder, dome, cone, and pyramid. We have simulated various structures and investigated the shape dependent optical properties using open source simulation tool available on the NanoHub platform. This simulation tool can simulate the simple as well as multilayer zero-dimensional structures by solving Schrödinger equations. The results suggested that the energy states vary according to the shape and higher energy states are observed for cone-shaped whereas, cuboid shape shows lower energy states for zero-dimensional structure. Furthermore, optical simulation study suggested that the cuboid and cylinder shapes show maximum absorption whereas, minimum absorption is observed for the dome-shape. The higher absorption is due to the higher surface area of cuboid and cylinder shape, whereas, the insufficient polarization angle of the incident light lowers the absorption for the dome shape structure. Furthermore, the absorption property is not significantly altered during different temperature environments. The integrated absorption results suggested that the cuboid and cylinder shapes have higher absorption whereas, minimum integrated absorption is observed for the cone and pyramid shape zero-dimensional structures. The present results pave the way towards optimization of various parameters of quantum dot for optoelectronic applications.

**Keywords:** Quantum dot; Optical properties; GaAs; Simulation.

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## 1. INTRODUCTION

The quantum dot is a zero-dimensional semiconductor material which is tightly confined either by electrons or holes. In view of this, it is generally referred to as an artificial atom [1]. It is an intermediate system and possesses combined properties of bulk semiconductor and atoms. It is well-known fact that the band gap increases from bulk to nanoparticles. This is due to the fact that the small size produces stronger confinement and results in larger separation in electronics levels. Furthermore, it exhibits quantum mechanical properties and hence it is a potential candidate for the development of high-performance optoelectronic devices [2].

In recent years, quantum dots have been studied extensively by theory as well as experimental research groups. Recently, quantum-dot cellular automata were used to design novel in-memory computing architecture [3-4]. Furthermore, it can harness the power of quantum computing [5]. Additionally, properties of zero-dimensional structures could be used for optoelectronic device applications. Recently, Wu et al. demonstrated the nanocavity laser [6]. In the field of energy conversion devices, it can be used to increase the efficiency of the solar cell [7]. Yang et al. have developed red, green and blue LEDs structures and achieve the more than 10 % external quantum efficiency [8]. In many applications, the shape and size of the nanostructures matter a lot. In view of this, Sabaeian et al. have studied the size-dependent inter sub-band optical properties of dome-shaped InAs/GaAs quantum zero-dimensional structures [9]. In many device level applications, semiconductor low dimensional structures are generally used, particularly GaAs is the first choice for practical applications. The GaAs is an III-V compound semiconductor with atomic density ~ $4.5 \cdot 10^{22}$ atoms/cm$^3$, band gap ~ 1.42 eV and electron mobility ~ 400 cm$^3$/V-S.

The reported novel and exotic properties of nanostructures arise due to the quantum confinement effects. In addition to this, quantum confinement effects are strongly related to the size and shape [10]. The optical properties can be tuned by altering the electronic state, symmetry of wave functions, polarizations, and localization of electronic states. Engineering the size and shape is one of the ways to harness the excellent properties of nanomaterials for practical applications [10]. Considering this in mind, In the present work, we have simulated various GaAs quantum zero-dimensional structures and studied the shape dependent optical properties. The results of the present investigation are useful for the various optoelectronic applications.

## 2. COMPUTATIONAL DETAILS

In the present investigation, we have used 'Quantum Dot Lab', which is available on the NanoHub platform [11]. This tool can simulate the simple as well as multilayer structures. It can solve up to 20 eigenenergy states of the system by solving Schrödinger equations. Furthermore, one can simulate the various shapes such as cylinder, cuboid, cone, pyramid, and dome. We can

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tune the various parameters such as a number of states, shapes, dimensions, lattice constant, effective mass and energy gap in order to find out the physical dynamics of low dimensional nanostructures. Table 1 summarized the simulation parameters used in the present investigation.

**Table 1** – Simulation parameters of the present study

| Sr. No. | Simple Zero Dimensional Structure | |
|---|---|---|
| | Parameters | Chosen values with units |
| 1. | STRUCTURAL | |
| I | Number of quantum dots | 5 |
| II | Shapes | Cylinder, Cuboid, Cone, Pyramid, Dome |
| III | X-Dimension | 10 nm |
| IV | Y-Dimension | 10 nm |
| V | Z-Dimension | 10 nm |
| VI | Lattice constant | 0.526 nm |
| VII | Effective mass | 0.067 |
| VIII | Energy gap | 1.443 eV |
| 2. | OPTICAL | |
| A | Light polarization | $<\theta = 45°$ , $<\Phi = 0°$ |
| B | Absorption | |
| I | Absolute fermi level | NO |
| II | Electron fermi level | 0 eV |
| III | Temperature | 300 K |
| IV | State broadening | 0.01 |
| C | SWEEP | |
| I | Sweep parameters | The temperature in units of 'K' |
| II | Minimum | 1 K |
| III | Maximum | 400 K |
| IV | Number of points | 10 |

## 3. RESULTS AND DISCUSSION

It is well-known fact that the zero-dimensional structures have discrete electronic states and due to this reason, they are popular for the optoelectronic applications. In the present study, we have varied the shape by keeping eigenstate and Z-dimension constant. The effect of the shape on the 3D wave functions of the cuboid, cylinder, dome, cone, and pyramid shapes are shown in Fig. 1. Furthermore, the effect of the shape on the energy states is summarized in Table 2. In the present case, we have selected the 5 eigenstates for the simulation. Furthermore, the size of the Z-dimension was 10 nm. It is observed that the energy states are altered according to the shape. It is observed that the cone-shaped possess higher energy states than other shapes. In addition to this, cuboid shape shows lower energy states than its other counterparts [12].

The shape dependent optical property (absorption) is shown in Figs. 2a, 2b. These results are obtained by simulating the different structures at 1 K and 400 K temperature, respectively. It is observed that the cuboid and cylinder structures show maximum absorption than the cone and pyramid shapes. The increase in the absorption is due to the higher surface area of cuboid and cylinder nanostructures. In addition to this, minimum absorption is observed for the dome shape nanostructure. The decrease in the absorption for dome shape is due to the insufficient polarization angle of the incident light [13]. It is observed that the absorption becomes constant at higher energy for all nanostructures. Furthermore, the absorption property is not significantly altered during 1 K and 400 K temperature environments. In order to understand the effect of the temperature, we have calculated the integrated absorption, as shown in Fig. 3a. The integrated absorption plot for different nanostructures suggested that the absorption is constant throughout the temperature range (1 K to 400 K). In other words, ambient temperature does not affect the absorption

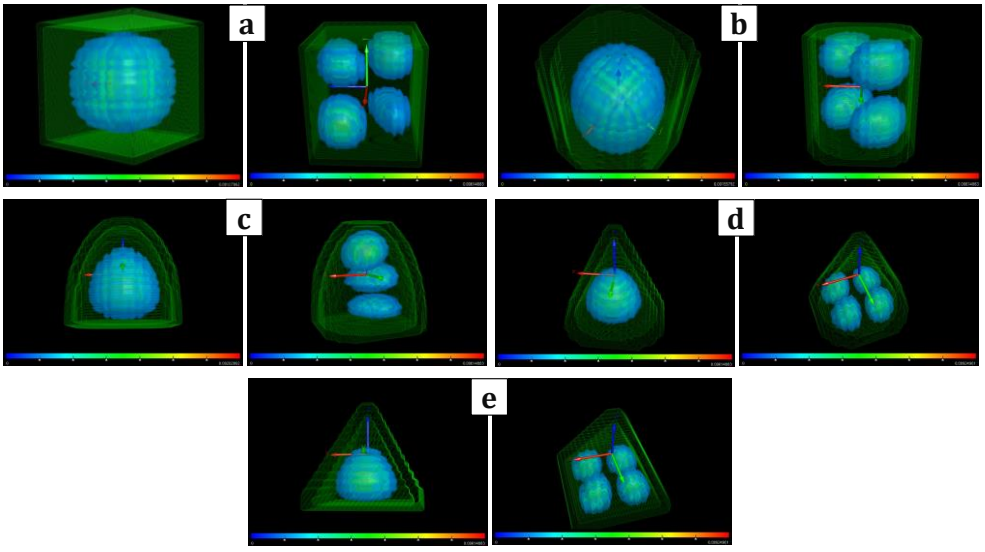


**Fig. 1** – 3D wave functions (ground and excited state) of (a) cuboid, (b) cylinder, (c) dome, (d) cone, (e) pyramid shaped quantum dots

**Table 2** – Shape dependent energy state properties

| Sr. No. | Shape | Energy States, eV | | | | |
|---|---|---|---|---|---|---|
| | | Ground State | 1st Excited State | 2nd Excited State | 3rd Excited State | 4th Excited State |
| 1 | Cuboid | 1.6120 | 1.7920 | 1.7920 | 1.7920 | 1.9719 |
| 2 | Cylinder | 1.6366 | 1.8166 | 1.8544 | 1.8616 | 2.0343 |
| 3 | Dome | 1.7109 | 1.9598 | 1.9935 | 1.9994 | 2.3007 |
| 4 | Cone | 1.9582 | 2.4206 | 2.4255 | 2.4475 | 2.9416 |
| 5 | Pyramid | 1.9248 | 2.3393 | 2.3399 | 2.3979 | 2.7103 |

property. Furthermore, integrated absorption results suggested that the cuboid and cylinder shapes have higher absorption than their other counterparts. The minimum integrated absorption is observed for the cone and pyramid nanostructures. The integrated absorption results suggested that the dome shape have moderate absorption. This kind of results appears during the temperature sweeping mode and is absent for the light polarization sweeping mode. In order to confirm this behavior, we have simulated the different nanostructures at $\Phi = 0°$ and $\theta = 45°$, as shown in Fig. 3 (b). The results clearly suggested that the absorption abruptly increases for the dome shape. The increase in the absorption for dome shape is due to the correct angle between incident light and a target. When the light is incident at the correct angle, it is strongly absorbed. When polarised light strikes to the surface of different shapes, it absorbs differently. In view of this, absorption strongly depends on the shape of the gallium arsenide quantum dots.

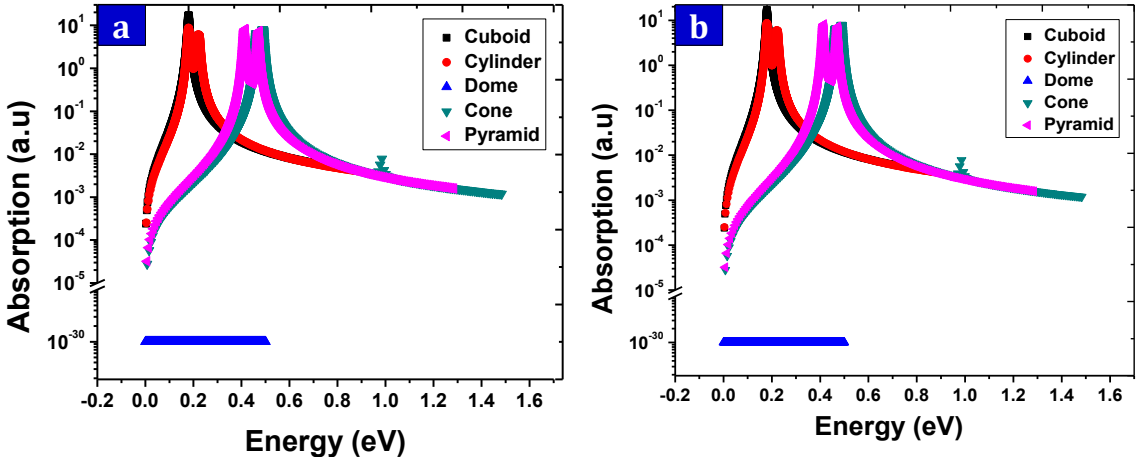


**Fig. 2** – Absorption of polarized light at (a) 1 K and (b) 400 K temperature

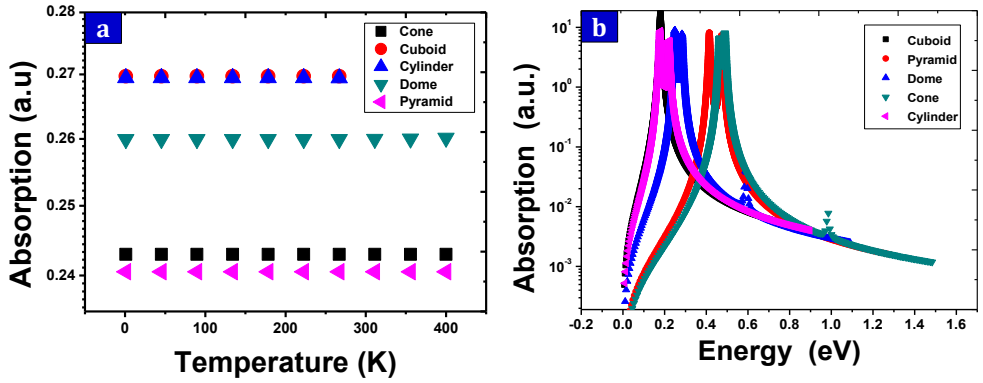


**Fig. 3** – (a) Integrated absorption at various temperature; (b) Absorption of light at $\Phi = 0°$, $\theta = 45°$

## 4. CONCLUSIONS

In this paper, shape dependent optical properties of GaAs quantum dots are investigated. It is observed that the energy states varied according to the shape of the zero-dimensional structures. In particular, the cone shape possesses higher energy states, whereas, the cuboid shape shows lower energy states. In the case of the absorption, the cuboid and cylinder shapes show maximum absorption due to higher surface area whereas, minimum absorption is observed for the dome shape due to the insufficient polarization angle of the incident light. Moreover, the absorption becomes constant at higher energy for all nanostructures. It is observed that the absorption property not significantly altered during 1 K and 400 K temperature environ-

ments. The integrated absorption results suggested that the cuboid and cylinder shapes have higher absorption whereas, minimum integrated absorption is observed for the cone and pyramid shapes. The results clearly suggested that the absorption property strongly depends on the shape of the nanostructure. The results of the present investigation are useful for the various optoelectronic applications such as light emitting diodes, solar cells, UV detectors, and display devices.

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## Залежні від форми оптичні властивості квантової точки GaAs: модельне дослідження


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У роботі розглянуто моделювання квантової точки GaAs з різними формами, такими як кубічна, циліндрична, куполоподібна, конусоподібна і пірамідальна. Проведено моделювання різних структур і досліджено оптичні властивості в залежності від форми квантової точки, використовуючи інструмент моделювання з відкритим вхідним кодом, доступний на платформі NanoHub. За його допомогою можна моделювати як прості, так і багатошарові структури нульової розмірності, розв'язуючи рівняння Шредінгера. Отримані результати свідчать про те, що енергетичні стани змінюються в залежності від форми квантової точки, для конусоподібних точок спостерігаються більш високі енергетичні стани. Крім того, моделювання показало, що кубічна і циліндрична форми мають максимальне поглинання, тоді як мінімальне поглинання спостерігається для куполоподібної форми. Більш високе поглинання відбувається за рахунок більшої площі поверхні кубічної і циліндричної форм, тоді як недостатній кут поляризації падаючого світла знижує поглинання для структури куполоподібної форми. Крім того, поглинальна властивість суттєво не змінюється при різних температурах середовища. Результати інтегрованого поглинання показали, що кубічна і циліндрична форми мають більш високе поглинання, тоді як мінімальне поглинання спостерігається для конусоподібної і пірамідальної форм структур нульової розмірності. Наведені результати відкривають шлях до оптимізації різних параметрів квантової точки для оптоелектронних приладів.



**Ключові слова:** Квантова точка; Оптичні властивості; GaAs; Моделювання.