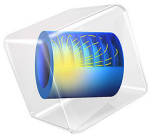


Model created in COMSOL Multiphysics 6.4

Conical Quantum Dot

This application computes the electronic states for a quantum-dot/wetting-layer system. It was inspired largely by the work of Dr. M. Willatzen and Dr. R. Melnik (Ref. 1) as well as B. Lassen.

Introduction

Quantum dots are nanoscale or microscale devices created by confining free electrons in a 3D semiconducting matrix. The tiny islands or droplets of confined "free electrons" (those with no potential energy) present many interesting electronic properties. They are of potential importance for applications in quantum computing, biological labeling, and lasers, to name only a few.

Scientists can create such structures experimentally using the Stranski-Krastanow molecular beam-epitaxy technique. In that way they obtain 3D confinement regions (the quantum dots) by growth of a thin layer of material (the wetting layer) onto a semiconducting matrix. Quantum dots can have many geometries including cylindrical, conical, or pyramidal. This application studies the electronic states of a conical InAs quantum dot grown on a GaAs substrate.

To compute the electronic states taken on by the quantum dot/wetting layer assembly embedded in the GaAs surrounding matrix, you must solve the 1-band Schrödinger equation in the effective mass approximation:

$$-\frac{h^2}{8\pi^2}\left(\nabla\cdot\left(\frac{1}{m_e(r)}\nabla\Psi(r)\right)\right)+V(r)\Psi(r)=E\Psi(r)$$

where h is the Planck constant, Ψ is the wave function, E is the eigenvalue (energy), and m_e is the effective electron mass (to account for screening effects).

Model Definition

The model works with the 1-particle stationary Schrödinger equation

$$-\nabla\cdot\left(\frac{h^2}{8\pi^2 m}\nabla\Psi\right)+V\Psi=E\Psi$$

It solves this eigenvalue problem for the quantum-dot/wetting-layer system using the following step potential barrier and effective-mass approximations:

- $V = 0$ for the InAs quantum dot/wetting layer and $V = 0.697$ eV for the GaAs substrate.
- $m_e = 0.023m$ for InAs and $m_e = 0.067m$ for GaAs.

Assume the quantum dot has perfect cylindrical symmetry. In that case you can model the overall structure in 2D as shown in the following figure.

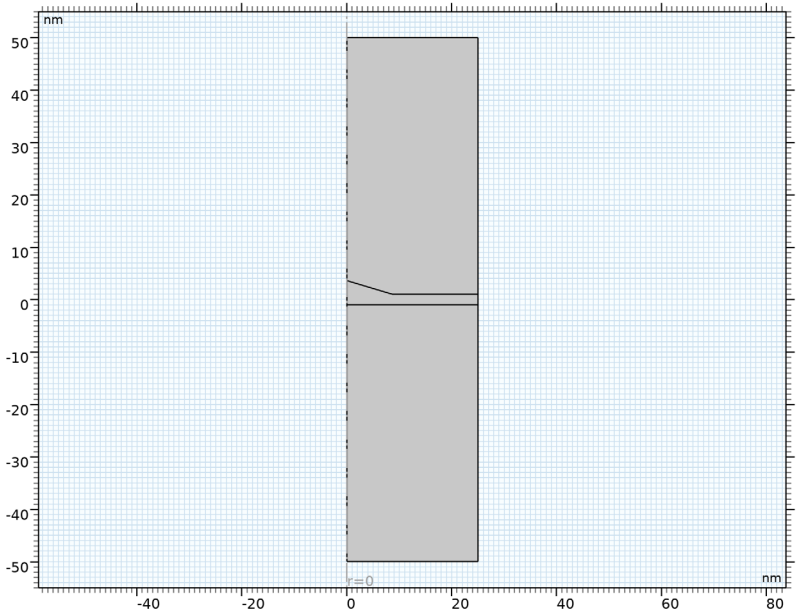


Figure 1: 2D geometry of a perfectly cylindrical quantum dot and wetting layer.

You can now separate the total wave function Ψ into

$$\Psi = \chi(z, r)\Theta(\varphi)$$

where φ is the azimuthal angle. Then rewrite the Schrödinger equation in cylindrical coordinates as

$$-\frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e}\frac{\partial \chi}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e}\frac{\partial \chi}{\partial r}\right)\right]\Theta - \frac{h^2}{8\pi^2}\frac{\chi}{m_e r^2}\frac{d^2\Theta}{d\varphi^2} + V\chi\Theta = E\chi\Theta$$

Dividing this equation by

$$\frac{\chi(z,r)}{m_e r^2}\Theta(\varphi)$$

and rearranging its terms lead to the two independent equations

$$\frac{1}{\Theta}\frac{d^2\Theta}{d\varphi^2} = -l^2 \tag{1}$$

and

$$-m_e r^2 \frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e}\frac{\partial \chi_l}{\partial z}\right)\frac{1}{\chi_l} + \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e}\frac{\partial \chi_l}{\partial r}\right)\frac{1}{\chi_l}\right] + m_e r^2[V-E] = -\frac{h^2}{8\pi}l^2 \tag{2}$$

Equation 1 has obvious solutions of the form

$$\Theta = \exp[il\varphi]$$

where the periodicity condition $\Theta(\varphi + 2\pi) = \Theta(\varphi)$ implies that l, the principal quantum number, must be an integer. It remains to solve Equation 2, which you can rewrite as

$$-\frac{h^2}{8\pi^2}\left[\frac{\partial}{\partial z}\left(\frac{1}{m_e}\frac{\partial \chi_l}{\partial z}\right) + \frac{1}{r}\frac{\partial}{\partial r}\left(\frac{r}{m_e}\frac{\partial \chi_l}{\partial r}\right)\right] + \left(\frac{h^2}{8\pi^2 m_e}\frac{l^2}{r^2} + V\right)\chi_l = E_l\chi_l, \qquad l \in \mathbf{Z}$$

Note that this is an instance of a PDE on coefficient form,

$$\nabla \cdot (-c\nabla u - \alpha u + \gamma) + au + \beta \cdot \nabla u = d_a \lambda u$$

where the nonzero coefficients are

$$c = \frac{h^2}{8\pi^2 m_e}, \qquad a = \frac{h^2}{8\pi^2 m_e}\frac{l^2}{r^2} + V, \qquad \beta_r = -\frac{h^2}{8\pi^2 m_e}\frac{1}{r}, \qquad d_a = 1$$

and $\lambda = E_l$.

Results

This exercise models the eigenvalues for the four lowest electronic energy levels for the principal quantum number $l = 0$. The plots in Figure 2 show the eigenwave functions for those four states.

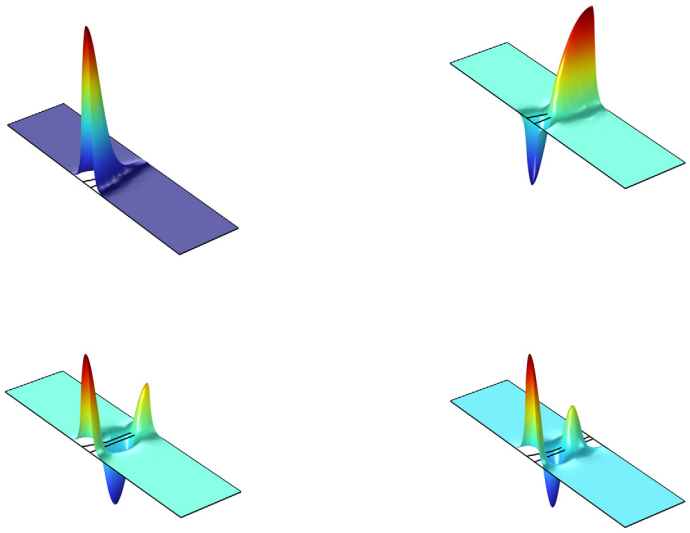


Figure 2: The four lowest electronic-energy levels for the case l = 0.

Notes About the COMSOL Implementation

To solve this problem, use the Coefficient Form PDE interface. The model solves for an eigenvalue/eigenfunction, for which you must input appropriate physical data and constants. Use electronvolts as the energy unit and nanometers as the length unit for the geometry.

Reference

1. R. Melnik and M. Willatzen, "Band structure of conical quantum dots with wetting layers," *Nanotechnology*, vol. 15, pp. 1–8, 2004.

Application Library path: `COMSOL_Multiphysics/Equation_Based/conical_quantum_dot`

Modeling Instructions

From the **File** menu, choose **New**.

NEW

In the **New** window, click **Model Wizard**.

MODEL WIZARD

1 In the **Model Wizard** window, click **2D Axisymmetric**.

2 In the **Select Physics** tree, select **Mathematics** > **PDE Interfaces** > **Coefficient Form PDE (c)**.

3 Click **Add**.

4 Click **Study**.

5 In the **Select Study** tree, select **General Studies** > **Eigenvalue**.

6 Click **Done**.

GLOBAL DEFINITIONS

Define dimensionless parameters for the electron mass and the reduced Planck constant expressed in electronvolt units. You can obtain these values by dividing the SI-unit values of the corresponding predefined COMSOL Multiphysics constants, `me_const` and `hbar_const`, by the value of the elementary charge `e_const` in coulombs.

Parameters 1

1 In the **Model Builder** window, under **Global Definitions** click **Parameters 1**.

2 In the **Settings** window for **Parameters**, locate the **Parameters** section.

3 In the table, enter the following settings:

Name	Expression	Value	Description
m	me_const[1/kg]/e_const[1/C]	5.6856E-12	Electron mass (eV/c^2)
hbar	hbar_const[1/(J*s)]/e_const[1/C]	6.5821E-16 rad	Reduced Planck constant (eV*s)
V_In	0	0	Potential barrier, InAs (eV)

Name	Expression	Value	Description
V_Ga	0.697	0.697	Potential barrier, GaAs (eV)
c_In	hbar^2/(2*0.023*m)	1.6565E-18 rad	c coefficient, InAs
c_Ga	hbar^2/(2*0.067*m)	5.6865E-19 rad	c coefficient, GaAs
l	0	0	Principal quantum number

GEOMETRY 1

1 In the **Model Builder** window, under **Component 1 (comp1)** click **Geometry 1**.

2 In the **Settings** window for **Geometry**, locate the **Units** section.

3 From the **Length unit** list, choose **nm**.

Rectangle 1 (r1)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type 25.

4 In the **Height** text field, type 100.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

6 In the **r** text field, type 12.5.

7 Click **Build Selected**.

Rectangle 2 (r2)

1 In the **Geometry** toolbar, click **Rectangle**.

2 In the **Settings** window for **Rectangle**, locate the **Size and Shape** section.

3 In the **Width** text field, type 25.

4 In the **Height** text field, type 2.

5 Locate the **Position** section. From the **Base** list, choose **Center**.

6 In the **r** text field, type 12.5.

7 Click **Build Selected**.

Polygon 1 (pol1)

1 In the **Geometry** toolbar, click **Polygon**.

2 In the **Settings** window for **Polygon**, locate the **Coordinates** section.

3 In the table, enter the following settings:

r (nm)	z (nm)
0	0
12	0
0	3.6

4 Click **Build Selected**.

Compose 1 (co1)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Compose**.

2 Select the objects **pol1** and **r2** only.

3 In the **Settings** window for **Compose**, locate the **Compose** section.

4 In the **Set formula** text field, type `r2+pol1`.

5 Clear the **Keep interior boundaries** checkbox.

6 Click **Build Selected**.

Compose 2 (co2)

1 In the **Geometry** toolbar, click **Booleans and Partitions** and choose **Compose**.

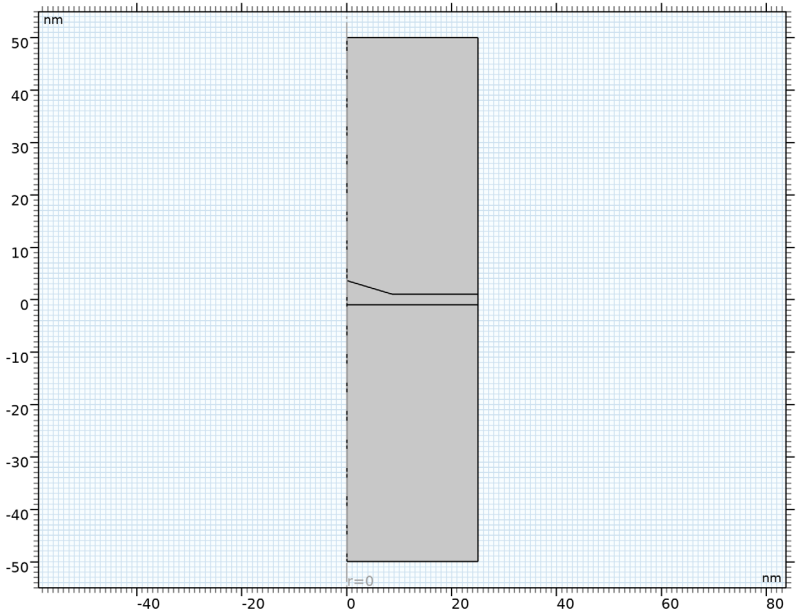
2 Click in the **Graphics** window and then press Ctrl+A to select both objects.

3 In the **Settings** window for **Compose**, locate the **Compose** section.

4 In the **Set formula** text field, type `r1+co1`.

5 Click **Build Selected**.

6 Click the **Zoom Extents** button in the **Graphics** toolbar.



COEFFICIENT FORM PDE (C)

Coefficient Form PDE 1

1 In the **Model Builder** window, under **Component 1 (comp1)** > **Coefficient Form PDE (c)** click **Coefficient Form PDE 1**.

2 In the **Settings** window for **Coefficient Form PDE**, locate the **Diffusion Coefficient** section.

3 In the *c* text field, type `c_In`.

4 Locate the **Absorption Coefficient** section. In the *a* text field, type `c_In*(1/r)^2+V_In`.

5 Click to expand the **Convection Coefficient** section. Specify the β vector as

`-c_In/r`	`r`
0	`z`

Coefficient Form PDE 2

1 In the **Physics** toolbar, click **Domains** and choose **Coefficient Form PDE**.

2 Select Domains 1 and 3 only.

3 In the **Settings** window for **Coefficient Form PDE**, locate the **Diffusion Coefficient** section.

4 In the *c* text field, type `c_Ga`.

5 Locate the **Absorption Coefficient** section. In the α text field, type `c_Ga*(1/r)^2+V_Ga`.

6 Click to expand the **Convection Coefficient** section. Specify the β vector as

`-c_Ga/r`	`r`
`0`	`z`

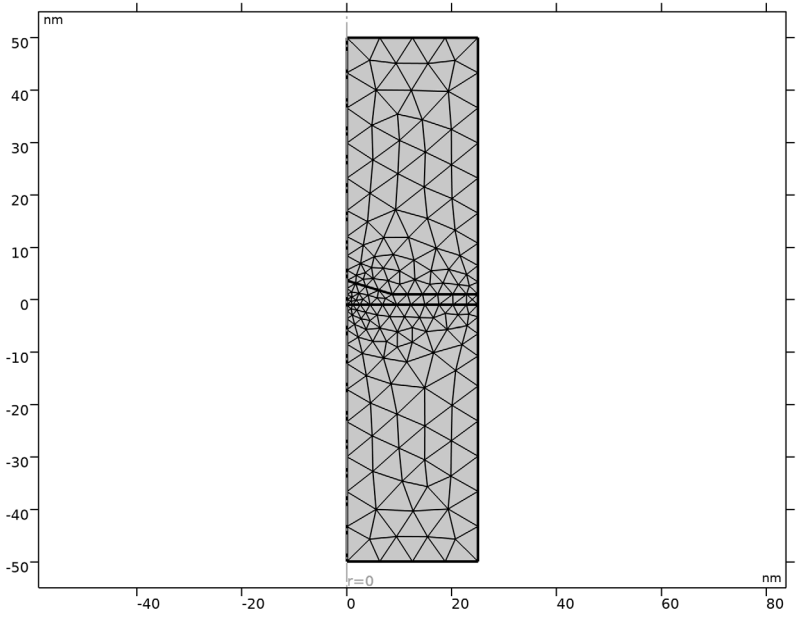
Dirichlet Boundary Condition 1

1 In the **Physics** toolbar, click **Boundaries** and choose **Dirichlet Boundary Condition**.

2 Select Boundaries 2 and 9 only.

MESH 1

In the **Model Builder** window, under **Component 1 (comp1)** right-click **Mesh 1** and choose **Build All**.



STUDY 1

Step 1: Eigenvalue

1 In the **Model Builder** window, under **Study 1** click **Step 1: Eigenvalue**.

2 In the **Settings** window for **Eigenvalue**, locate the **Study Settings** section.

3 Select the **Desired number of eigenvalues** checkbox. In the associated text field, type `4`.

4 In the **Study** toolbar, click **Compute**.

RESULTS

Follow the instructions below to reproduce the series of plots in Figure 2.

Height Expression 1

1 In the **Model Builder** window, expand the **Results** > **Coefficient Form PDE** node.

2 Right-click **Surface 1** and choose **Height Expression**.

3 Click the **Zoom Extents** button in the **Graphics** toolbar.

Compare the result to the upper-left plot in Figure 2.

Coefficient Form PDE

1 In the **Model Builder** window, under **Results** click **Coefficient Form PDE**.

2 In the **Settings** window for **2D Plot Group**, locate the **Data** section.

3 From the **Eigenvalue (rad/s)** list, choose **0.3932**.

4 In the **Coefficient Form PDE** toolbar, click **Plot**.

5 Click the **Zoom Extents** button in the **Graphics** toolbar.

Compare the result to the upper-right plot in Figure 2.

6 From the **Eigenvalue (rad/s)** list, choose **0.45891**.

7 In the **Coefficient Form PDE** toolbar, click **Plot**.

8 Click the **Zoom Extents** button in the **Graphics** toolbar.

Compare the result to the lower-left plot in Figure 2.

9 From the **Eigenvalue (rad/s)** list, choose **0.5653**.

10 In the **Coefficient Form PDE** toolbar, click **Plot**.

11 Click the **Zoom Extents** button in the **Graphics** toolbar.

Compare the result to the lower-right plot in Figure 2.