Density of States:
2D, 1D, and 0D

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Introduction

The density of states function describes the number of states that are available in a system and is essential for determining the carrier concentrations and energy distributions of carriers within a semiconductor.

In semiconductors, the free motion of carriers is limited to two, one, and zero spatial dimensions. When applying semiconductor statistics to systems of these dimensions, the density of states in quantum wells (2D), quantum wires (1D), and quantum dots (0D) must be known.

Derivation of Density of States (2D)

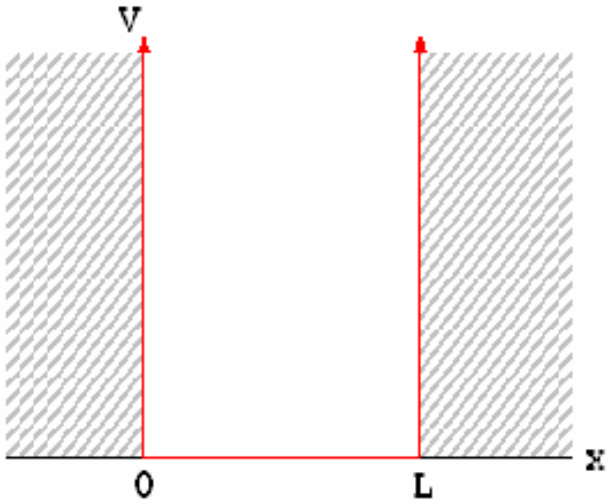
We can model a semiconductor as an infinite quantum well (2D) with sides of length L. Electrons of mass m* are confined in the well.

If we set the PE in the well to zero, solving the Schrödinger equation yields

$$\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi = E\psi$$

$$\frac{\partial^2\psi}{\partial x^2}+\frac{\partial^2\psi}{\partial y^2}+k^2\psi = 0 \qquad \text{(Eq. 1)}$$

$$where\ \ k=\sqrt{\frac{2mE}{\hbar^2}}$$



Derivation of Density of States (2D)

Using separation of variables, the wave function becomes

$$\psi(x,y) = \psi_x(x)\psi_y(y) \qquad \text{(Eq. 2)}$$

Substituting Eq. 2 into Eq. 1 and dividing through by $\psi_x\psi_y$ yields

$$\frac{1}{\psi_x}\frac{\partial^2\psi}{\partial x^2} + \frac{1}{\psi_y}\frac{\partial^2\psi}{\partial y^2} + k^2 = 0 \qquad \text{where k= constant}$$

This makes the equation valid for all possible x and y terms only if terms including $\psi_x(x) \quad and \quad \psi_y(y)$ are individually equal to a constant.

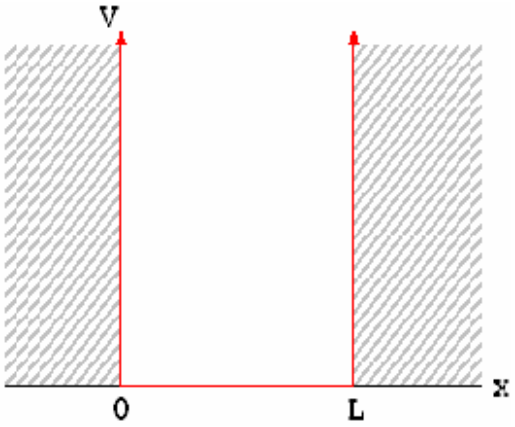
Derivation of Density of States (2D)

Thus,

$$\frac{1}{\psi_x}\frac{\partial^2\psi}{\partial x^2} = -k^2$$

where $k^2 = k_x^2 + k_y^2$

$$\frac{1}{\psi_y}\frac{\partial^2\psi}{\partial y^2} = -k^2$$



The solutions to the wave equation where $V(x) = 0$ are sine and cosine functions

$$\psi = A\sin(k_x x) + B\cos(k_x x)$$

Since the wave function equals zero at the infinite barriers of the well, only the sine function is valid. Thus, only the following values are possible for the wave number (k):

$$k_x = \frac{n_x\pi}{L}, \quad k_y = \frac{n_y\pi}{L} \quad for\ n = \pm 1, 2, 3....$$

Derivation of Density of States (2D)

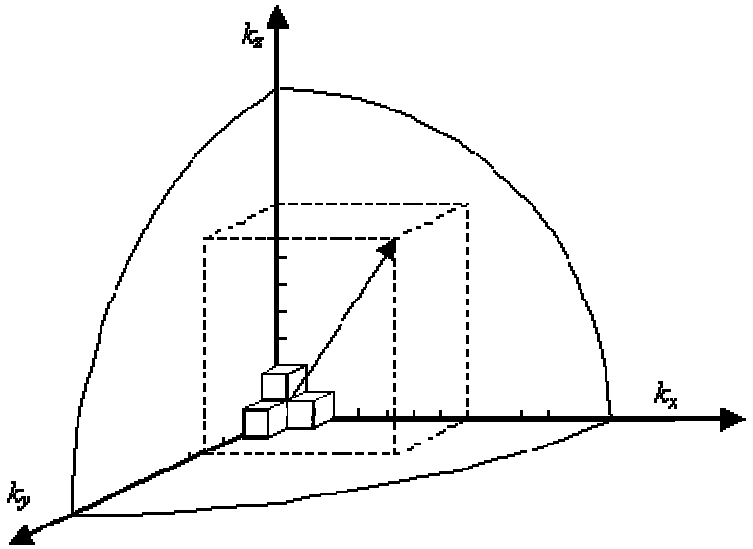
Recalling from the density of states 3D derivation…

k-space volume of single state cube in k-space:

$$V_{single-state} = \left(\frac{\pi}{a}\right)\left(\frac{\pi}{b}\right)\left(\frac{\pi}{c}\right) = \left(\frac{\pi^3}{V}\right)$$

k-space volume of sphere in k-space:

$$V_{sphere} = \frac{4\pi k^3}{3}$$



$$where\ k = \sqrt{\frac{2mE}{\hbar^2}}$$

V is the volume of the crystal.
$V_{single-state}$ is the smallest unit in k-space and is required to hold a single electron.

Derivation of Density of States (2D)

Recalling from the density of states 3D derivation…

k-space volume of single state cube in k-space: $V_{single-state} = \left(\frac{\pi}{a}\right)\left(\frac{\pi}{b}\right)\left(\frac{\pi}{c}\right) = \left(\frac{\pi^3}{V}\right) = \left(\frac{\pi^3}{L^3}\right)$

k-space volume of sphere in k-space: $V_{sphere} = \frac{4\pi k^3}{3}$

Number of filled states in a sphere: $N = \frac{V_{Sphere}}{V_{single-state}} \times 2 \times \left(\frac{1}{2} \times \frac{1}{2} \times \frac{1}{2}\right)$

$$N = \frac{\frac{4}{3}\pi k^3}{\frac{\pi^3}{L^3}} \times 2 \times \left(\frac{1}{8}\right) = \frac{4\pi k^3 L^3}{3\pi^2}$$

A factor of two is added to account for the two possible electron spins of each solution.

Correction factor for redundancy in counting identical states +/- n_x, +/- n_y, +/- n_z

Derivation of Density of States (2D)

For calculating the density of states for a 2D structure (i.e. quantum well), we can use a similar approach, the previous equations change to the following:

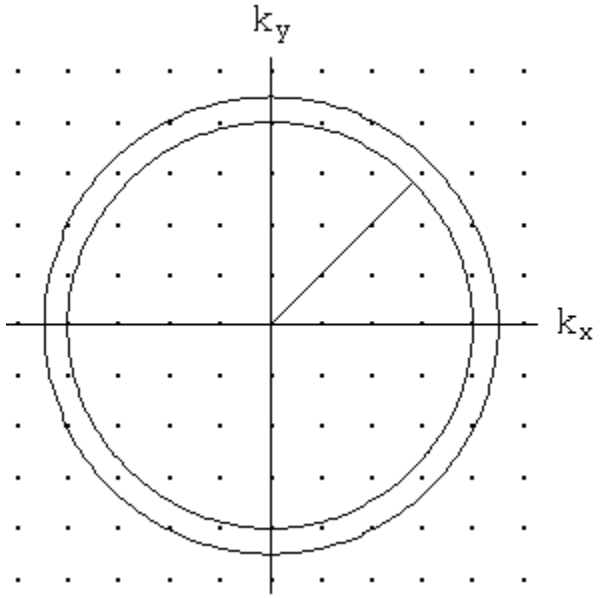
k-space volume of single state cube in k-space: $V_{\sin gle-state} = \left(\frac{\pi}{a}\right)\left(\frac{\pi}{b}\right) = \left(\frac{\pi^2}{V}\right) = \left(\frac{\pi^2}{L^2}\right)$

k-space volume of sphere in k-space: $V_{circle} = \pi k^2$

Number of filled states in a sphere:

$$N = \frac{V_{circle}}{V_{\sin gle-state}} \times 2 \times \left(\frac{1}{2} \times \frac{1}{2}\right)$$

$$N = \frac{\pi k^2}{\frac{\pi^2}{L^2}} \times 2 \times \left(\frac{1}{4}\right) = \frac{k^2 L^2}{2\pi}$$



Derivation of Density of States (2D)

continued……

$$N = \frac{k^2 L^2}{2\pi},$$

Substituting $k = \sqrt{\frac{2mE}{\hbar^2}}$ yields

$$\Downarrow$$

$$N = \frac{\left(\sqrt{\frac{2mE}{\hbar^2}}\right)^2 L^2}{2\pi} = \frac{mL^2 E}{\hbar^2 \pi}$$

The density per unit energy is then obtained using the chain rule:

$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = \frac{L^2 m}{\pi\hbar^2}$$

Derivation of Density of States (2D)

The density of states per unit volume, per unit energy is found by dividing by V (volume of the crystal).

$g(E)_{2D}$ becomes:

$$g(E)_{2D=} \frac{\frac{L^2 m}{\pi\hbar^2}}{L^2} = \frac{m}{\pi\hbar^2}$$

As stated initially for the electron mass, $m \longrightarrow m^*$.

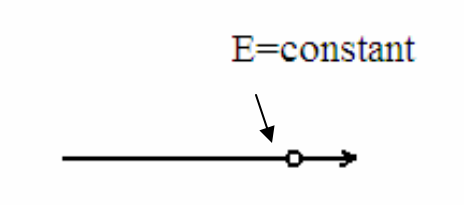
Thus,

$$g(E)_{2D} = \frac{m^*}{\pi\hbar^2}$$

It is significant that the 2D density of states does not depend on energy. Immediately, as the top of the energy-gap is reached, there is a significant number of available states.

Derivation of Density of States (1D)

For calculating the density of states for a 1D structure (i.e. quantum wire), we can use a similar approach. The previous equations change to the following:



k-space volume of single state cube in k-space: $V_{single-state} = \left(\frac{\pi}{a}\right) = \left(\frac{\pi}{V}\right) = \left(\frac{\pi}{L}\right)$

k-space volume of sphere in k-space: $V_{line} = k$

$$N = \frac{V_{line}}{V_{single-state}} \times 2 \times \left(\frac{1}{2}\right)$$

Number of filled states in a sphere:

$$N = \frac{k}{\frac{\pi}{L}} = \frac{kL}{\pi}$$

Derivation of Density of States (1D)

Continued….. $N = \dfrac{kL}{\pi}$, Substituting $k = \sqrt{\dfrac{2mE}{\hbar^2}}$ yields

$$N = \frac{\sqrt{\dfrac{2mE}{\hbar^2}}L}{\pi} = \sqrt{2mE}\,\frac{L}{\hbar\pi}$$

Rearranging…… $N = (2mE)^{1/2}\,\dfrac{L}{\hbar\pi}$

The density per unit energy is then obtained by using the chain rule:

$$\frac{dN}{dE} = \frac{dN}{dk}\frac{dk}{dE} = \frac{\frac{1}{2}(2mE)^{-1/2}\cdot 2mL}{\hbar\pi} = \frac{(2mE)^{-1/2}\cdot mL}{\hbar\pi}$$

Derivation of Density of States (1D)

The density of states per unit volume, per unit energy is found by dividing by V (volume of the crystal).

$g(E)_{1D}$ becomes:

$$g(E)_{1D} = \frac{\frac{(2mE)^{-1/2} \cdot mL}{\hbar\pi}}{L} = \frac{(2mE)^{-1/2} \cdot m}{\hbar\pi} = \frac{m}{\hbar\pi\sqrt{2mE}}$$

Simplifying yields…

$$g(E)_{1D=} \frac{m}{\hbar\pi\sqrt{2mE}} \cdot \frac{\sqrt{m}}{\sqrt{m}}$$

$$g(E)_{1D=} \frac{1}{\hbar\pi} \cdot \sqrt{\frac{m}{2E}}$$

Derivation of Density of States (1D)

As stated initially for the electron mass, $m \longrightarrow m^*$. Also, because only kinetic energy is considered $E \longrightarrow Ec$.

Thus,

$$g(E)_{1D} = \frac{1}{\hbar\pi} \cdot \sqrt{\frac{m^*}{2(E - E_c)}}$$

Derivation of Density of States (0D)

When considering the density of states for a 0D structure (i.e. quantum dot), no free motion is possible. Because there is no k-space to be filled with electrons and all available states exist only at discrete energies, we describe the density of states for 0D with the delta function.

Thus,

$$g(E)_{0D} = 2\delta(E - E_c)$$

Additional Comments

The density of states has a functional dependence on energy.

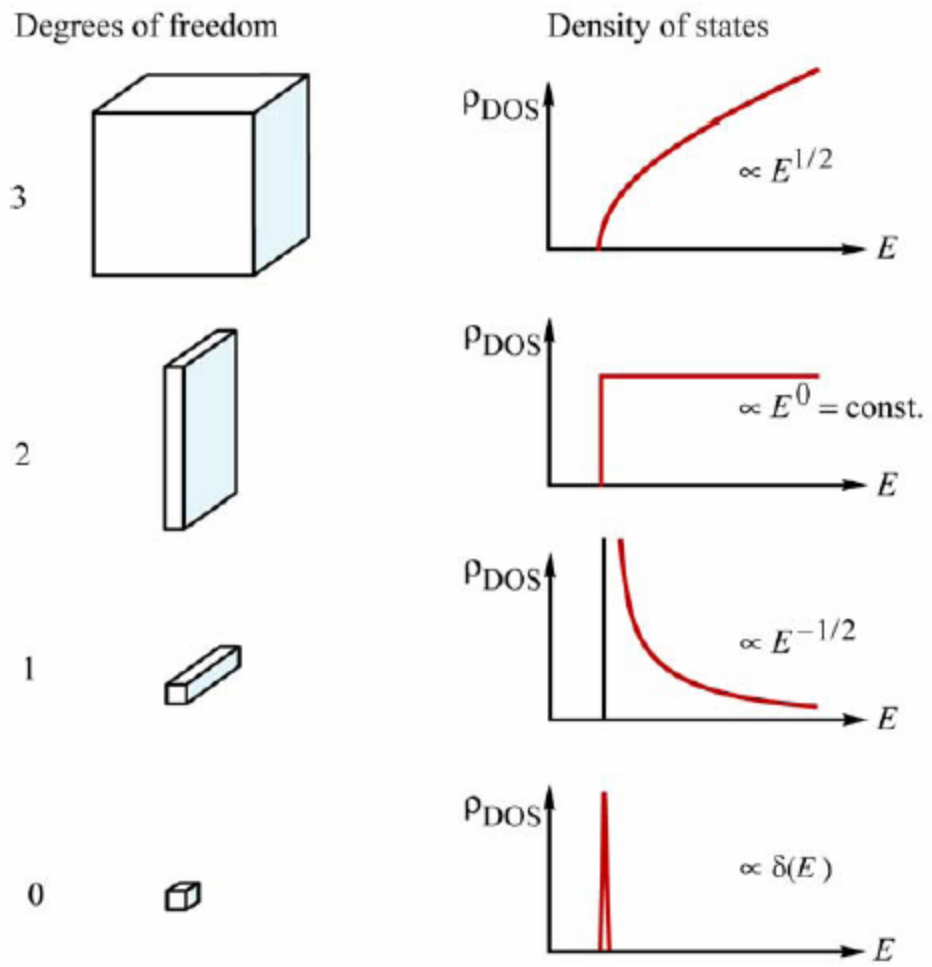


Fig. 12.7. Electronic density of states of semiconductors with 3, 2, 1, and 0 degrees of freedom for electron propagation. Systems with 2, 1, and 0 degrees of freedom are referred to as quantum wells, quantum wires, and quantum boxes, respectively.

Additional Comments

Degrees of freedom	Dispersion (kinetic energy)	Density of states	Effective density of states
3 (bulk)	$E = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2 + k_z^2)$	$\rho_{DOS}^{3D} = \frac{1}{2\pi^2}\left(\frac{2m^*}{\hbar^2}\right)^{\frac{3}{2}}\sqrt{E - E_C}$	$N_c^{3D} = \frac{1}{\sqrt{2}}\left(\frac{m^* kT}{\pi\hbar^2}\right)^{\frac{3}{2}}$
2 (slab)	$E = \frac{\hbar^2}{2m^*}(k_x^2 + k_y^2)$	$\rho_{DOS}^{2D} = \frac{m^*}{\pi\hbar^2}\sigma(E - E_C)$	$N_c^{2D} = \frac{m^*}{\pi\hbar^2}kT$
1 (wire)	$E = \frac{\hbar^2}{2m^*}(k_x^2)$	$\rho_{DOS}^{1D} = \frac{m^*}{\pi\hbar}\sqrt{\frac{m^*}{2(E - E_C)}}$	$N_c^{1D} = \sqrt{\frac{m^* kT}{2\pi\hbar^2}}$
0 (box)	–	$\rho_{DOS}^{0D} = 2\delta(E - E_C)$	$N_c^{0D} = 2$

Table 12.1 Density of states for semiconductor with 3, 2, 1, and 0 degrees of freedom for propagation of electrons. The dispersion relations are assumed to be parabolic. The formulas can be applied to anisotropic semiconductors if the effective mass m^* is replaced by the density-of-states effective mass m_{DOS}^*. If the semiconductor has a number of M_c equivalent minima, the corresponding density of states must be multiplied by M_c. The bottom of the band is denoted as E_C and $\sigma(E)$ is the step-function.

Practical Applications

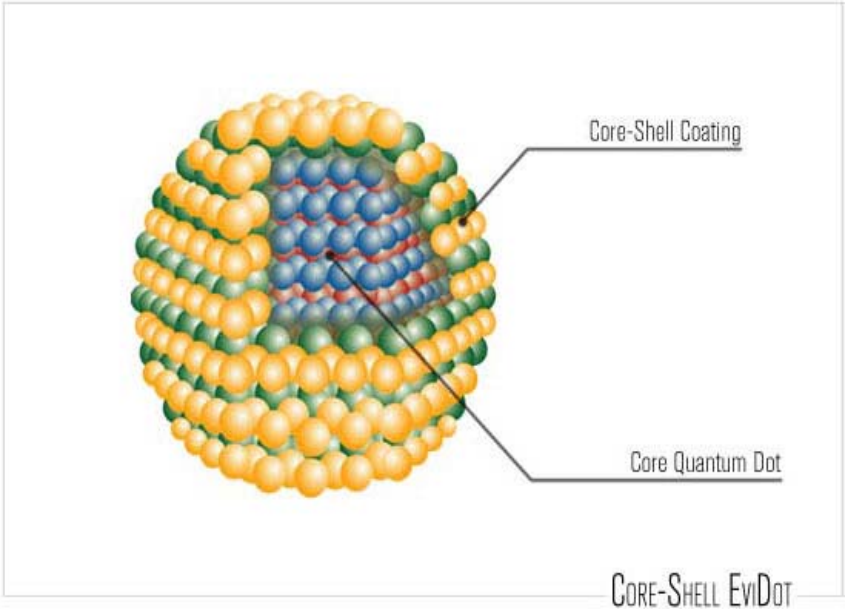
Quantum Wells (2D) - a potential well that confines particles in one dimension, forcing them to occupy a planar region

Quantum Wire (1D) - an electrically conducting wire, in which quantum transport effects are important

Quantum Dots (0D) - a semiconductor crystal that confines electrons, holes, or electron-pairs to zero dimensions.

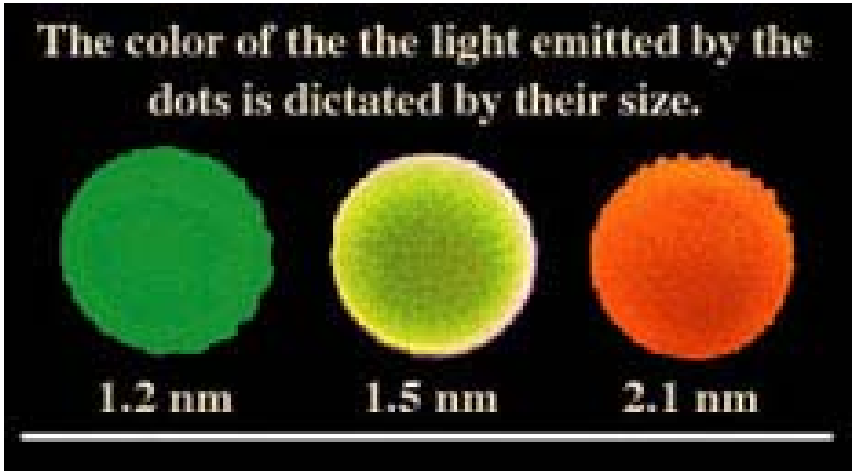
Quantum Dots

- Small devices that contain a tiny droplet of free electrons.
- Dimensions between nanometers to a few microns.
- Contains single electron to a collection of several thousands
- Size, shape, and number of electrons can be precisely controlled



Quantum Dots

- Exciton: bound electron-hole pair (EHP)
- Attractive potential between electron and hole
- Excitons generated inside the dot
- Excitons confined to the dot
  - Degree of confinement determined by dot size
  - Discrete energies



Fabrication Methods

- Goal: to engineer potential energy barriers to confine electrons in 3 dimensions

- 3 primary methods
  - Lithography
  - Colloidal chemistry
  - Epitaxy

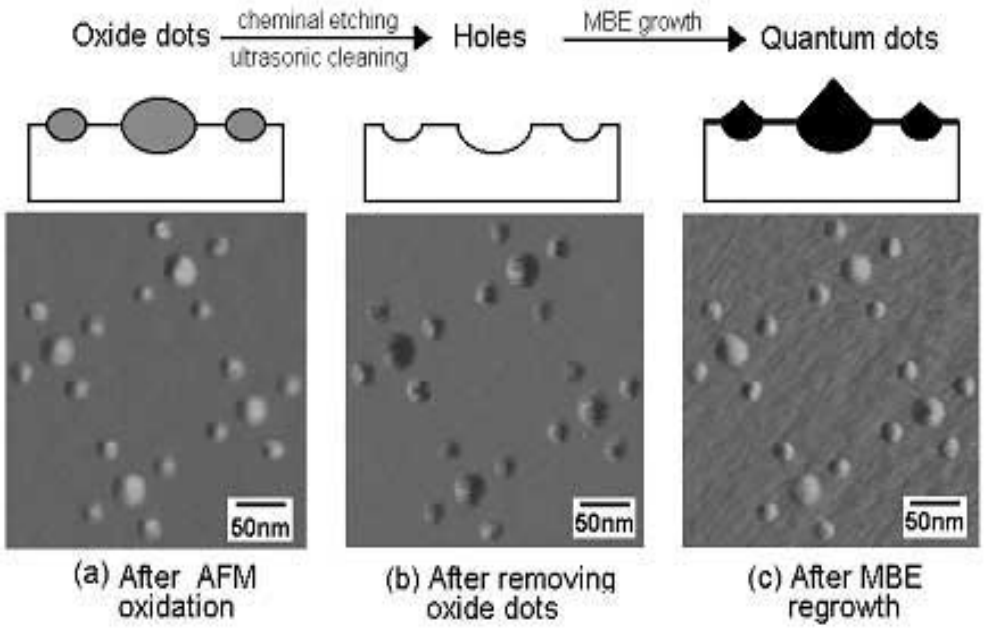
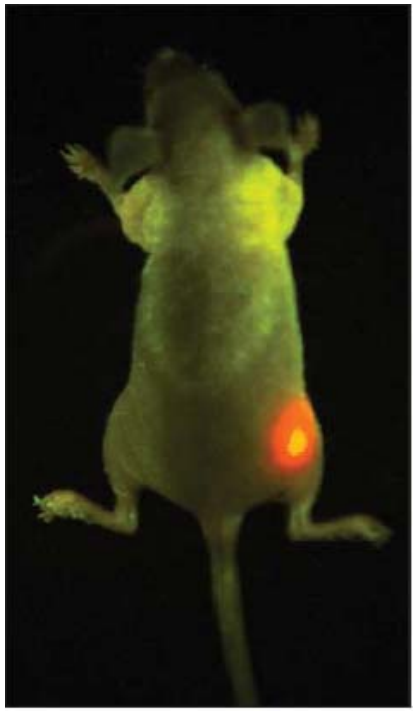


FIG. 1 Quantum dot fabrication processes and array of fabricated quantum dots

Future Research

- Probe fundamental physics
- Quantum computing schemes
- Biological applications
- Improved Treatments for Cancer
- Optical and optoelectronic devices, quantum computing, and information storage.
- Semiconductors with quantum dots as a material for cascade lasers.
- Semiconductors with quantum dots as a material for IR photodetectors
- Injection lasers with quantum dots
- Color coded dots for fast DNA testing
- 3-D imaging inside living organisms



Bull's-eye. Red quantum dots injected into a live mouse mark the location of a tumor.

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