

Quantum wells

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It is well known that electronic and optical properties can be altered by using heterostructures and the most widely used heterostructures in semiconductors are quantum wells. When semiconductors are fabricated in sufficiently thin layers, quantum interference effects begin to appear prominently in the motion of the electrons, as a result of the quantum confinement of the carriers in the resulting one-dimensional potential wells. The quantum well, in which a single layer of one narrow-gap semiconductor is sandwiched between two layers of a wider-gap material, is illustrated in Fig.1 [1]. In such a quantum well heterostructure, the confinement can change the optical adsorption from the smooth function, as in a bulk material, to a series of steps. The confinement can also increase the binding energy of excitons, resulting in exceptionally clear excitonic resonances at room temperature in quantum well heterostructures. Thus, quantum well hetero-structures are key components of many electronic and optoelectronic devices, because they can increase the strength of electro-optical interactions by confining the carriers to small regions.

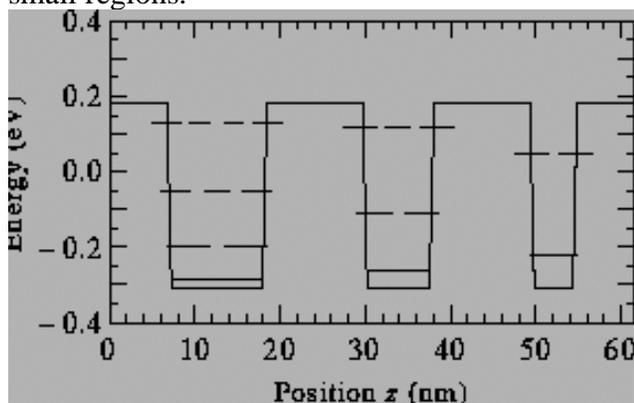


FIG. 1 Energy-band profile of a structure containing three quantum wells, showing the confined states in each well. The structure consists of GaAs wells of thickness 11, 8, and 5 nm in $\text{Al}_{0.4}\text{Ga}_{0.6}\text{As}$ barrier layers. The gaps in the lines indicating the confined state energies show the locations of nodes of the corresponding wavefunctions.

In order to get a good sense of the quantum well heterostructures, in addition to the electronic and optoelectronic properties of such semiconductor structures, we should begin from some basic concepts.

From electron transfer theory, the electrons are restricted to a finite region of space, denoted a “quantum well” or a “particle in a box.” The simplest example is the infinitely deep “square” well and is illustrated in Fig. 2. Within this well, the electron has zero potential energy in the region $0 < x < L$, and infinitely high potential barriers prevent it from straying beyond this region. Note that L is the full width of the well here.

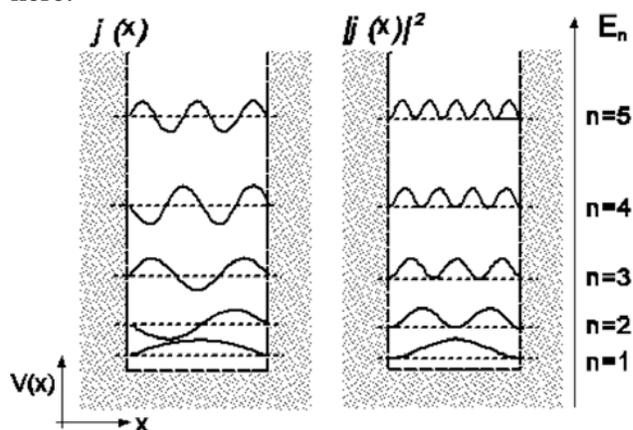


FIG. 2 Energy levels and wave functions for an infinitely deep square potential well

The Schrödinger equation for motion inside the well is identical to that for free space:

$$-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} = E\psi(x) \quad (1)$$

The boundary conditions are

$$\psi = 0 \text{ for } x = 0 \quad (2)$$

$$\psi = 0 \text{ for } x = L \quad (3)$$

We could use real trigonometric functions and write

$$\psi = A \cdot \sin(kx) \quad (4)$$

Where

$$k = (2m_e E)^{1/2} / \hbar \quad (5)$$

and m_e is the mass of the electron.

Substitution shows that the function is a solution with

$$E = \frac{\hbar^2 k^2}{2m} \equiv \varepsilon_0(k) \quad (6)$$

$$\text{Hence, } kL = n\pi, \quad (7)$$

That is:

$$E = \frac{\hbar^2 k^2}{2m_e} = \frac{\hbar^2}{2m_e} \cdot \left(\frac{\pi n}{L}\right)^2 \quad (8)$$

Or

$$E = E_n = \frac{\pi^2 \hbar^2 n^2}{2m_e L^2} \quad (9)$$

Where n is a quantum number with the value of any positive integer. As we have solved the above wave function and corresponding energy value in our first problem set, so I will skip some details in the above calculation. The normalization constant, A , can be found from the probability of finding a particle in the box:

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx = \int_0^L \left| A \sin\left(\frac{\pi n}{L} x\right) \right|^2 dx = 1 \quad (10)$$

This condition means that the particle is localized within the potential well, so that the probability of finding the particle in the potential well is equal to unity.

$$\int_0^L \left| A \sin\left(\frac{\pi n}{L} x\right) \right|^2 dx = |A|^2 \int_0^L \left| \sin\left(\frac{\pi n}{L} x\right) \right|^2 dx = \frac{|A|^2}{2} \int_0^L [1 - \cos(2\frac{\pi n}{L} x)] dx = 1 \quad (11)$$

Using above equation, we obtain $A = \sqrt{\frac{2}{L}}$.

Hence,

$$\psi_n(x) = \left(\frac{2}{L}\right)^{1/2} \sin\left(\frac{\pi n}{L} x\right) \quad (12)$$

In fact, an infinitely deep well cannot be made, but it has become routine to grow structures that are close to ideal finite wells. Now we consider how Fig. 2 changes if the potential at the walls is not infinite.

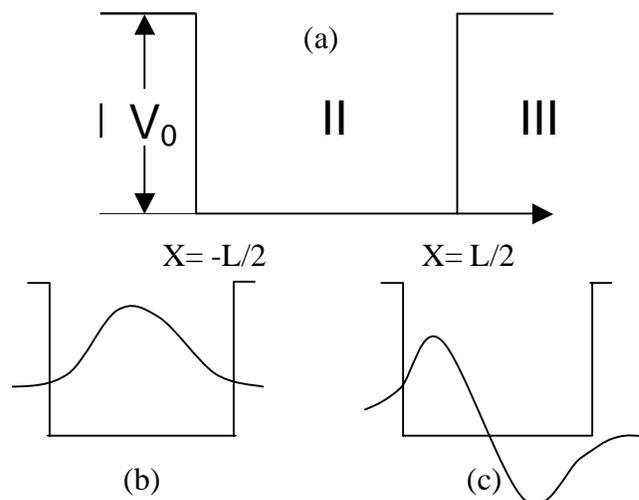


FIG. 3 (a) Potential energy for a particle in a one-dimensional finite rectangular well; (b) The ground-state wave function for this potential; (c) The first excited-state wave function.

It will turn out to be convenient to have the origin at the center of the well, so we take

$$V(x) = V_0 \text{ for } x < -L/2 \quad (13)$$

$$V(x) = 0 \text{ for } -L/2 < x < L/2 \quad (14)$$

$$V(x) = V_0 \text{ for } L/2 < x \quad (15)$$

There are two cases to examine, depending on whether the particle's energy E is greater than or smaller than the potential V_0 .

The Schrödinger equation for the barrier region I and III becomes:

$$\frac{\hbar^2}{2m} \frac{\partial^2 \psi(x)}{\partial x^2} + (E - V_0)\psi(x) = 0 \quad (16)$$

This is a linear homogenous differential equation with constant coefficients, and there are two exponential solutions outside the well (say, for x

> $L/2$) one increasing to the right, the other decreasing,

$e^{\alpha x}$ And $e^{-\alpha x}$, where

$$\alpha = \sqrt{2m(V_0 - E)/\hbar^2} \quad (17)$$

The wave function outside the well is: $\psi = Ae^{\alpha x} + Be^{-\alpha x}$, where A,B are constants. We are assuming here that $E < V_0$, so the particle is bound to the well. We shall find this is always true for the lowest energy state. Let us try to construct the wave function for the energy E corresponding to this lowest bound state. From the equation with $V_0 = 0$, the wave function inside the well (let's assume it's symmetric for now) is proportional to $\cos kx$, where $k = \sqrt{2mE/\hbar^2}$.

The wave function and its derivative inside the well must match a sum of exponential terms—the wave function in the *wall*—at $x = L/2$, so

$$\begin{aligned} \cos(kL/2) &= Ae^{\alpha L/2} + Be^{-\alpha L/2} \\ -k \sin(kL/2) &= \alpha Ae^{\alpha L/2} - \alpha Be^{-\alpha L/2} \end{aligned} \quad (18)$$

The *only* exponential wave function that makes sense is the one for which A is *exactly zero*. It can also be confirmed because the quantity $\sqrt{V_0 - E}$ is a real, positive number, and to keep the wave function far away from the wall finite, we must have $A=0$. Thus there is only a *decreasing* wave in the wall. Requiring the decreasing wave function, $A = 0$, means that only a discrete set of values of k , or E , satisfy the boundary condition equations above. They are most simply found by taking $A = 0$ and dividing one equation by the other to give:

$$\tan(kL/2) = \alpha / k \quad (19)$$

This can be solved graphically by plotting the two sides as functions of k and find where the curves intersect.

We can also see from the above equations that only the particular values of E give a wave function that is continuous and has a continuous

derivative, so the energy levels are quantized for $E < V_0$. The particular values of E are given by:

$$(2E - V_0) \sin[(2mE)^{1/2} L/\hbar] = 2(V_0 E - E^2)^{1/2} \cos[(2mE)^{1/2} L/\hbar] \quad (20)$$

Here, we are not going to talk in detail about the derivation of above equation. You can try it if you are interested.

Let's go back to the Fig.3, which shows the wave function for the lowest two energy levels. The wave function is oscillatory inside the well and dies off exponentially outside the well. It turns out that the number of nodes increases by one for each higher level. And states with $E < V_0$ are bound.

So far, we have considered only states with $E < V_0$. For $E > V_0$, the quantity $\sqrt{V_0 - E}$ becomes imaginary. By repeating the same procedures as for the case of $E < V_0$, however, this time, we cannot set A as zero. With this additional constant, the energy E need not be restricted to obtain properly behaved wave functions, because A and B can match each other. Therefore, all energies above V_0 will be allowed and states with $E > V_0$ are unbound. For the particles in an infinitely deep well, all the states are bound.

Currently, there is great scientific and technological interest in quantization effects in semiconductor structures. The underlying reason is that the optical, electrical and photoredox properties of semiconductors can be tuned and manipulated in fascinating ways by controlling dimension, rather than by controlling composition alone. Interest in the alloying of two materials to reach an objective is due to the fact that: 1) because the band gap determines the energy of light emitted and absorbed, which is essential in the laser/detector area, alloying can create a desired band gap; 2) it is possible to create a material with a proper lattice constant to match or mismatch with an available substrate. The widely studied semiconductor heterostructures are GaAs/AlAs largely because GaAs and AlAs are nearly lattice matched so that the alloy can be grown on GaAs substrate without strain energy build-up. Here we will examine the case of GaAlAs as an example [2].

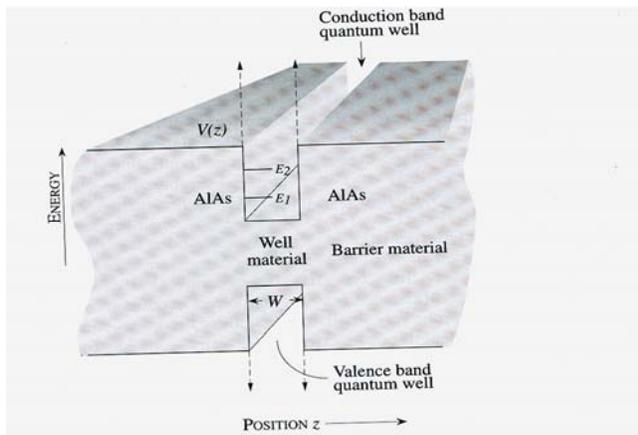


FIG. 4 A schematic of a quantum well formed for the electron and holes in a heterostructure

The Schrödinger equation for the electron states in the quantum well can be written in a simple approximation as:

$$-\frac{\hbar^2}{2m^*} \frac{d^2\psi}{dx^2} + V\psi(x) = E\psi(x) \quad (21)$$

Where m^* is the effective mass of the electron, with a unit of kg.

We can obtain exactly the same results as discussed above; we just need to replace the mass of a particle by the effective mass of the electron. We can see that each level of energy is actually a subband due to the electron energy in the x - y plane. The subband structure has important consequences for optical and transport properties of heterostructures. However, the density of states (DOS) of the electronic band will be an important manifestation of this subband. Now, we will use electron transfer theory to study the quantum wells^[3].

First, we look at the behavior of the electrons. Free electrons have energy $\epsilon_0(k) = \hbar^2 k^2 / 2m_0$ (m_0 is the bulk mass). Electrons in a semiconductor are in the conduction band, and this fact leads to changes in their energy in two ways. First, energy must be measured from the bottom of the band at E_c rather than from zero. Second, electrons behave as though their mass is m^* ,

Where the effective mass is defined by analogy with Newton's second law of motion:

$$F = m^* \frac{dv}{dt} \quad (v \text{ is the velocity of electron with the}$$

unit of m/s). In GaAs the effective mass m_e is $0.067 m_0$. Thus $\epsilon_0(k) = E_c + \hbar^2 k^2 / 2m^*$. The sandwich acts like a quantum well because E_c is higher in AlGaAs than in GaAs, and the difference ΔE_c provides the barrier that confines the electrons. Typically $\Delta E_c \approx 0.2 - 0.3 eV$, a value that is not large. However, we shall approximate it as infinite to find the energy levels in a well of width a . Adapting equation shows that the energy of the bound states, labeled with n_e , is

$$\epsilon_{en_e} \approx E_c^{GaAs} + \frac{\hbar^2 \pi^2 n_e^2}{2m^* a^2} \quad (22)$$

Semiconductors have energy levels in other bands. The most important of these is the valence band which lies below the conduction band. The top of this is at E_v and the band curves downwards as a function of k , giving $\epsilon_v(k) = E_v - \hbar^2 k^2 / 2m^{*}$, which contains another effective mass m^{*} ($m^{*} = 0.5m_0$ in GaAs). The conduction and valence bands are separated by an energy called the band gap given by $E_g = E_c - E_v$. Because E_v is at a different level in GaAs well and AlGaAs barriers, there is a quantum well. The energies of the bound states are

$$\epsilon_{hn_h} \approx E_v^{GaAs} - \frac{\hbar^2 \pi^2 n_h^2}{2m^{*} a^2} \quad (23)$$

In a pure semiconductor at zero temperature, the valence band is completely filled, and the conduction band is completely empty. Optical absorption excites an electron from the valence band into the conduction band, and an empty state or "hole" will be left in the valence band.

Now we will look at the quantum well^[4]. The lowest energy at which absorption can occur is given by the difference in energy $\epsilon_{e1} - \epsilon_{h1}$ between the lowest state in the well in the conduction band and the valence band. Absorption can occur at higher energies by using other states, and strong transitions occur between corresponding states in the two bands.

If the wells were really infinitely deep there would be an infinite series of lines with frequencies given by equation:

$$\lambda_{W_n} = \varepsilon_{em} - \varepsilon_{hm} = (E_c^{GaAs} + \frac{\hbar^2 \pi^2 n^2}{2m^* a^2}) - (E_v^{GaAs} - \frac{\hbar^2 \pi^2 n^2}{2m^* a^2}) = E_g^{GaAs} + \frac{\hbar^2 \pi^2 n^2}{2} (\frac{1}{m^*} + \frac{1}{m^*}) \quad (24)$$

The barriers in the semiconductor are finite, and absorption occurs in the AlGaAs barriers for all frequencies where $\hbar\omega > E_g^{AlGaAs}$ and it is impossible for adsorption for $\hbar\omega < E_g^{AlGaAs}$. So there is a discontinuity in the absorption spectrum. And there are two discrete lines produced by transitions between states in the quantum well lying between these two frequencies, $E_g^{AlGaAs} < \hbar\omega < E_g^{GaAs}$.

When electric fields are applied to bulk semiconductors, the band-edge adsorption broadens due to the Franz-Keldysh effect. When the effect of the Coulomb correlation of electron and hole is properly included, a Stark shift of the exciton resonance to lower energies is expected. However, for fields of the order of a few times the classical ionization field $E_i (=E_B/8ea, \text{ where } E_B \text{ is the zero-field binding energy and } a \text{ is the Bohr radius})$, the resonance is severely broadened because the field ionization drastically reduces the exciton life-time and the resonance shift is limited to $\sim 20\%$ of the binding energy.

Applications: Light Emitters

Heterostructures have multiple advantages over homo-p-n-junctions, regarding the parameters of light emitting diodes (LEDs) and laser diodes (LDs). The LEDs and LDs are both very important technology devices with application in displays and communications, including optical communications, optical memories, optical logic switches and lighting. The advances in these areas are coming from low-dimensional systems (quantum wells for example) and new materials. The LED is essentially a forward biased p-n diode. Electrons and holes are injected as minority carriers across the diode junction and they recombine either by radiative recombination or non-radiative recombination.

When the active region is made of a material with a narrower gap than that of the material through which radiation is emitted, loss of light in passive regions of the structure is reduced, and the loss is lowered by carrier recombination in emitters. These advantages were first actualized in AlGaAs heterostructure LEDs, in which a nearly 100% internal quantum efficiency of radiative recombination was achieved.

The laser diode, where quantum well heterostructures are always employed, acts the same way as LEDs. However, the laser structure is designed to create an optical "cavity" which can guide the photons generated. An important parameter of the laser cavity is the optical confinement factor Γ , which gives the fraction of the optical wave in the active region. This confinement factor is almost unity for bulk double heterostructure lasers where the active region is larger than 1.0 micron, while it is as small as 1% for advanced quantum well lasers. However, in spite of the small value of Γ , quantum well lasers have superior performance because of their superior electronic properties owing to their 2-dimensional density of states.

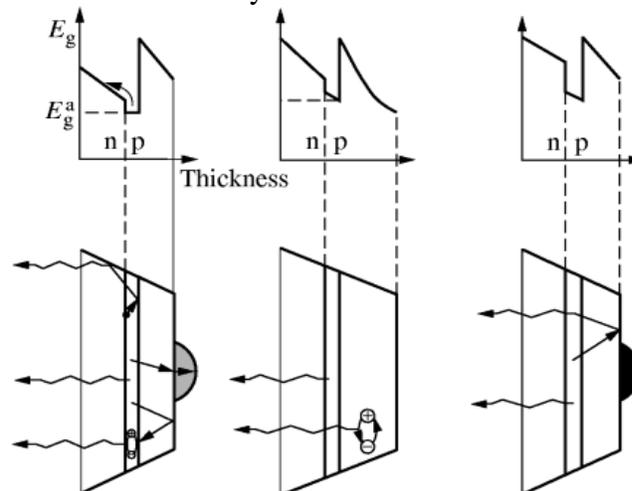


FIG. 5 Forbidden gap width in AlGaAs/GaAs heterostructure LEDs of three types and schematic of light reflection and "re-emission" processes.

Heterostructure Solar Cells and Photo-detectors

$A_{III}B_V$ heterostructure solar cells can be used to produce solar batteries with higher efficiency and radiation hardness. An important advantage

of heterostructure photoelectric converters is their ability to efficiently convert strongly concentrated (up to 1000–2000-fold) sunlight, which opens up possibilities of reducing significantly (in proportion to the extent of concentration) the area and cost of solar cells and, as a result, making "solar" electric power cheaper. MOCVD-grown heterostructure solar cells with built-in Bragg mirrors are of particular interest and AlGaAs/GaAs heterostructure solar cells are widely used in space due to their higher efficiency and improved radiation hardness.

A_{III}B_V heterostructure materials and their solid solutions are widely used now in new types of photodetectors, GaAs/AlGaAs-based for the spectral region 0.3–0.9 μm range, InP/InGaAsP-based for the 1.0–1.6 μm range, and the GaInSbAs system for longer wavelengths (2.0–6.0 μm). It was shown that the use of heterojunctions in photodetectors not only enable the control over their spectral sensitivity region, but also makes it possible to increase the quantum efficiency and speed of photodetectors by bringing into coincidence the regions of light absorption and separation of nonequilibrium carriers, to reduce dark currents, and, in some cases, to control impact ionization processes.

We can expect the further exploring of the optical and magnetic properties the quantum well heterostructure could bring to us.

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