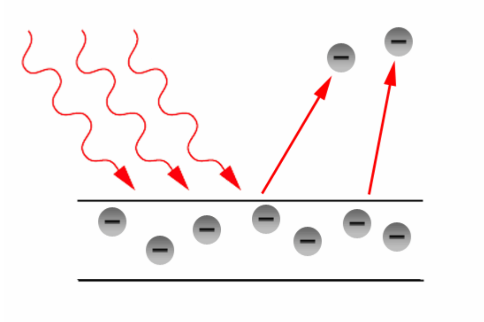
Quantum Description of Semiconductors

Quantum Mechanical Effects

Early experiments on black body radiation could not be explained by classical theory. Max Planck showed that energy could only be absorbed or emitted by in discrete amounts (called quanta, later called photons of light).



Photoelectric effect

Electrons emitted by photocathode only if $eV = hf + \phi$

Electron emission depends on the grid voltage. Intensity does not matter! –unlike classical theory.

Energy = h*f*   *where f* = frequency and h = Planck's constant

$\phi$is the work function – minimum energy required to extract an electron from photocathode. Any extra energy results in increased kinetic energy (speed) of emitted electron. The kinetic energy of the electron can be measured by increasing the grid voltage until no current flows.

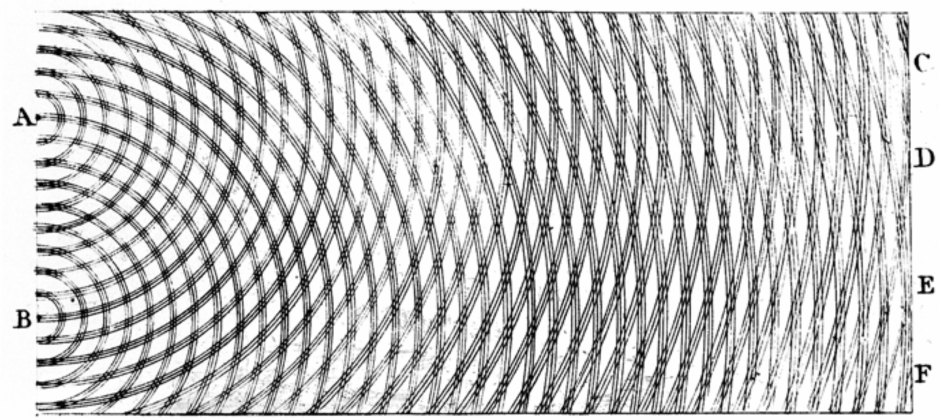
$$hf = e\varphi + eV_{stop} \qquad eV_{stop} = \frac{1}{2} m v_e^2$$

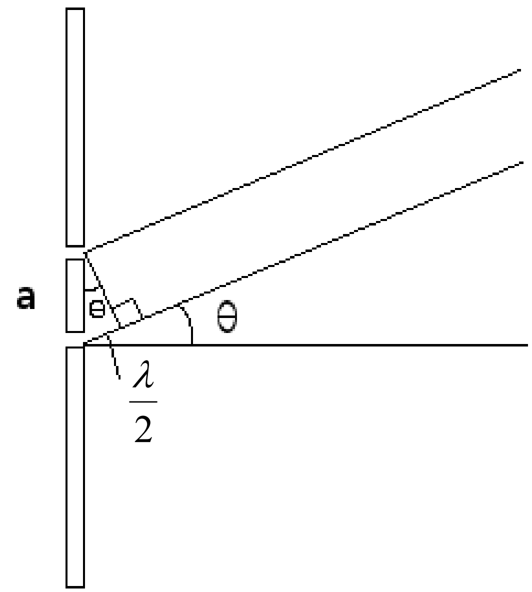
Light behaves like a **particle** of energy hf which can 'kick out' an electron particle from the solid

Diffraction

Demonstrates the wave like nature of light.

Consider diffraction from 2 slits: A and B

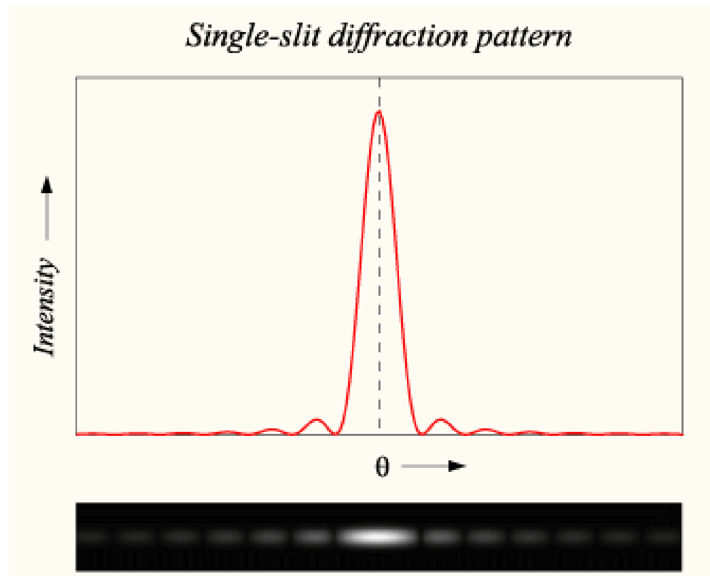




$$\text{maxima when } a\sin\theta = \lambda m$$

$$\text{minima when } a\sin\theta = \frac{\lambda}{2}(2m+1)$$

m is an integer that labels the *order* of each minimum,
λ is the wavelength,
a is the distance between the slits
and *θ* is the angle for destructive interference



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Wave Particle Duality

Photon energy, $E = hf$ Speed of light, $c = f\lambda$

If the photon energy E is transported at velocity ‘c’, its momentum $p = E/c$

Proof: I--dx--I F

• • ←

External force F acts on photon over distance dx, such that there is a change in photon energy, dE

$$\partial E = F\partial x \qquad F = \frac{\partial p}{\partial t}(\text{Newton}) \qquad \text{so } \partial E = \frac{\partial p \partial x}{\partial t} \qquad \partial E = c\partial p \qquad \text{Integrate } p = \frac{E}{c} = \frac{E}{f\lambda} = \frac{hf}{f\lambda} = \frac{h}{\lambda}$$

Photons (or any particles) with momentum p have an associated wavelength λ (de Broglie)

example 1: Apple (mass = 0.2kg) falls on ground with velocity 10m/s.
momentum $p = mv = 0.2 \times 10 = 2$kgm/s
associated $\lambda = h/p = 6.6 \times 10^{-34}/2 = 3.3 \times 10^{-34}$ m -this is a very, very short wavelength – impossible to measure, so treat as particle!

example 2: electron is accelerated through 100V.
Gain in K.E. = loss in P.E. $\frac{1}{2} mv^2 = eV$ $v = (2eV/m)^{\frac{1}{2}}$
momentum $p = mv = (2eVm)^{\frac{1}{2}}$ associated $\lambda = h/p = h(2eVm)^{-\frac{1}{2}} = 1.225\ V^{-\frac{1}{2}}$ nm
For 100V, $\lambda = 0.12$nm -this is measurable and useful (electron microscopes).

Quantum Description of Semiconductors

Wave versus particle dilemma can be addressed by thinking of the photon as a **wavepacket.** This is an envelope or packet containing an arbitrary number of wave forms. In quantum mechanics the wave packet is interpreted to be a "probability wave" describing the probability that a particle or particles in a particular state will have a given position and momentum

The Uncertainty Principle

To construct a wave packet representing a photon localised in a small region of space, the component waves must get out of phase rapidly. This means their wavelengths cannot be very close together. In fact, it is not difficult to give an estimate of the spread in wavelength necessary, just from a consideration of the two beating waves.

A packet localized in a region of extent Δx can be constructed of waves having k's spread over a range Δk, where $\Delta x \sim \pi / \Delta k$.

Now, $k = 2\pi / l$, and $p = h/l$, so $k = 2\pi p/h$.

$\Delta k = 2\pi \Delta p/h$, and $\Delta x \sim \pi / \Delta k \sim h/\Delta p$ (dropping the factor of 2).

Therefore $\Delta p.\Delta x=h$. Means if you know Δx to a very good accuracy we wont know Δp so accurately and vice versa

Quantum Description of Semiconductors

Particle in a quantum well

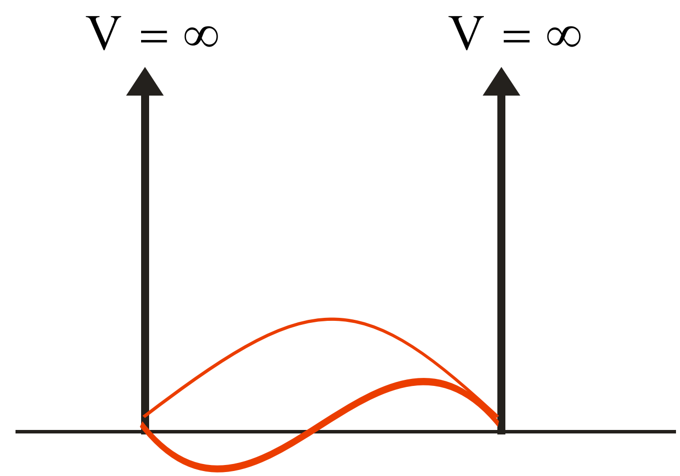
Assume that electron is bound by the well, i.e. it exists only within the well. Classical theory states that electron can have *any* energy within well.

As a wave however, only certain wavelengths (λ) are possible – those that fit between 0 and L.

$n\lambda/2 = L$ satisfies this requirement.

i.e. a whole number of ½ wavelengths must fit in the well.

$\lambda = 2L/n \quad E = p^2/2m = h^2/2m\lambda^2$



$$E_n = \frac{n^2 h^2}{8mL^2} \qquad n = 1,2,3....$$

i.e. electrons can only take up values given by En above - called **quantisation**. In most everyday cases, L is large (mm or larger) and E_n is very small. But for an electron confined between two atoms in a crystal, L = 1nm, E_n becomes significant

$$E = \frac{(6.6x10^{-24})^2}{8x9.1x10^{-21}x(10^{-9})^2} = 6.02x10^{-20} J = 0.38eV$$

Quantum Description of Semiconductors

Particle in a 1-dimensional box.

1D infinite square well with momentum only in the direction of quantum confinement (the *x* direction). The solution to this is called the1D time-independent Schrödinger equation can be written as:

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

where

$\hbar$ is the Reduced Planck Constant

m is the mass of the particle

$\psi(x)$ is the complex-valued stationary time-independent wavefunction that we want to find

$V(x)$ is the spatially varying potential and

E is the energy, a real number.

For the case of the particle in a 1-dimensional box of length *L*, the potential is zero inside the box, but rises abruptly to infinity at *x* = 0 and *x* = *L*. Thus for the region inside the box *V*(*x*) = 0 and Equation 1 reduces to:

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

The Potential is 0 inside the box, and infinite elsewhere. This is a well studied differential equation with a general solution of:

$$\psi(x)=A\sin(kx)+B\cos(kx) \qquad E=\frac{k^2\hbar^2}{2m} \quad (3)$$

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$$\psi(0) = \psi(L) = 0 \quad (4)$$

Substituting the general solution from Equation 3 into Equation 2 and evaluating at *x* = 0 (ψ = 0), we find that *B* = 0 (since sin(0) = 0 and cos(0) = 1). It follows that the wavefunction must be of the form:

$$\psi(x) = A\sin(kx) \quad (5)$$

and at *x* = *L* we find:

$$\psi(x) = A\sin(kL) = 0 \quad (6)$$

One solution for Equation 6 is *A* = 0, however, this "trivial solution" would imply that *ψ* = 0 everywhere (i.e. the particle isn't in the box.) and can be thrown out.

If $A \neq 0$ then sin(*kL*) = 0 only when: $k = \frac{n\pi}{l}$

And again $E_n = \frac{n^2h^2}{8mL^2} \qquad n = 1,2,3....$

In 2 dimensions $\psi_{n_x,n_y} = \sqrt{\frac{4}{L_xL_y}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right) \quad (E_{n_x,n_y} = \frac{\hbar^2\pi^2}{2m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2\right]$

In 3 dimensions

$$\psi_{n_x,n_y,n_z} = \sqrt{\frac{8}{L_xL_yL_z}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right)\sin\left(\frac{n_z\pi z}{L_z}\right) \quad E_{n_x,n_y,n_z} = \frac{\hbar^2\pi^2}{2m}\left[\left(\frac{n_x}{L_x}\right)^2 + \left(\frac{n_y}{L_y}\right)^2 + \left(\frac{n_z}{L_z}\right)^2\right]$$

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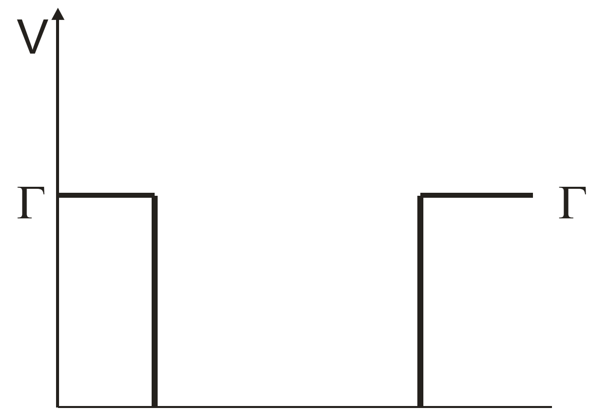

Particle in a FINITE quantum well

Inside the quantum well
and

$$\psi_2 = A\sin(kx) + B\cos(kx)$$

$$E = \frac{k^2\hbar^2}{2m}$$

Outside the quantum well
For the region outside of the box, $V(x) = \Gamma$ and Equation 1 becomes: $-\frac{\hbar^2}{2m}\frac{d^2\psi_1}{dx^2} = (E-\Gamma)\psi_1$

There are two possible families of solutions, depending on whether E is less than Γ (the particle is bound in the potential) or E is greater than Γ (the particle is free).
For a free particle, $E > \Gamma$, and letting

produces $\frac{d^2\psi_1}{dx^2} = -\kappa^2\psi_1$ $\quad \kappa = \frac{\sqrt{2m(E-\Gamma)}}{\hbar}$

with the same solution form as the inside-well case: $\psi_1 = C\sin(\kappa x) + D\cos(\kappa x)$

This analysis will first focus on the bound state, where $\Gamma > E$. letting $\alpha = \frac{\sqrt{2m(\Gamma - E)}}{\hbar}$
produces

$$\frac{d^2\psi_1}{dx^2} = \alpha^2\psi_1$$

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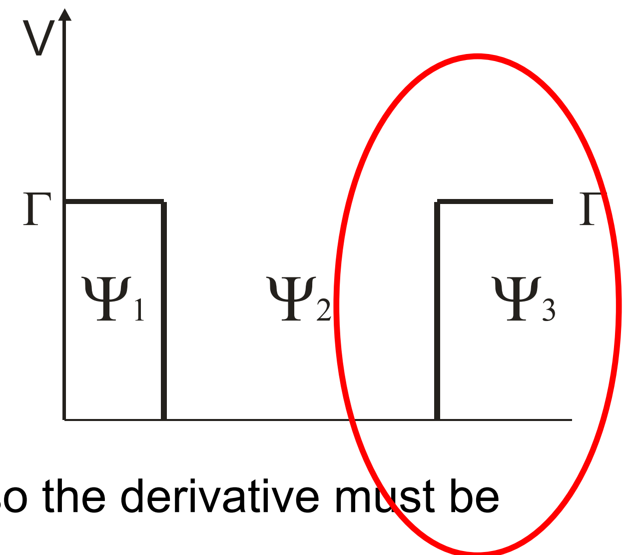
The general solution for this is an exponential: $\psi_1 = Fe^{-\alpha x} + Ge^{\alpha x}$

Similarly, for the other region outside the box: $\psi_3 = He^{-\alpha x} + Ie^{\alpha x}$



So we know have 3 wavefunctions: 1 in the quantum well and 2 outside

$$\psi_1 = Fe^{-\alpha x} + Ge^{\alpha x} \qquad \psi_2 = A\sin(kx) + B\cos(kx)$$

$$\psi_3 = He^{-\alpha x} + Ie^{\alpha x}$$

At the boundaries, the wavefunction must be continuous. Also the derivative must be continuous

$$\psi_1(-L/2) = \psi_2(-L/2) \qquad \psi_2(L/2) = \psi_3(L/2)$$

$$\frac{d\psi_1}{dx}(-L/2) = \frac{d\psi_2}{dx}(-L/2) \qquad \frac{d\psi_2}{dx}(L/2) = \frac{d\psi_3}{dx}(L/2)$$

Take a closer look at this region

The University Of Sheffield.

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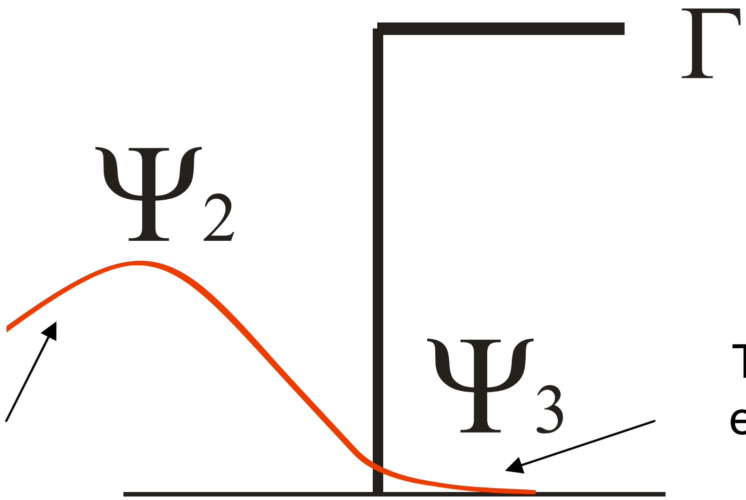
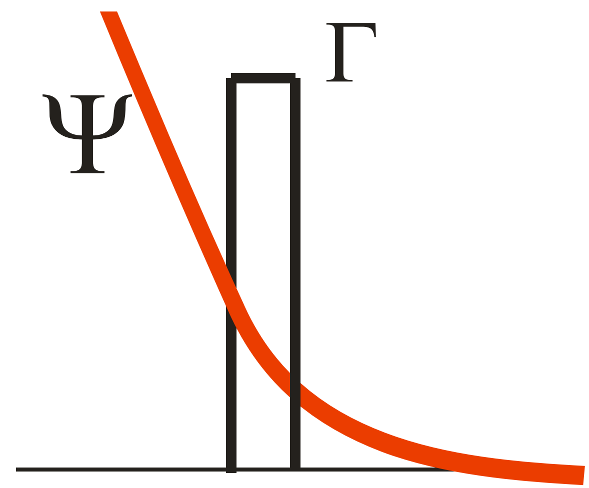
This needs to be sin(kx) function as before



This needs to be an exponential function

Note the wavefunction is not zero in the barrier anymore. This means there is some probability of electrons in the barrier

For a thin barrier, the wavefunction can penetrate through, giving a good probability of electrons on the right hand side. The phenomenon is called **Tunneling**



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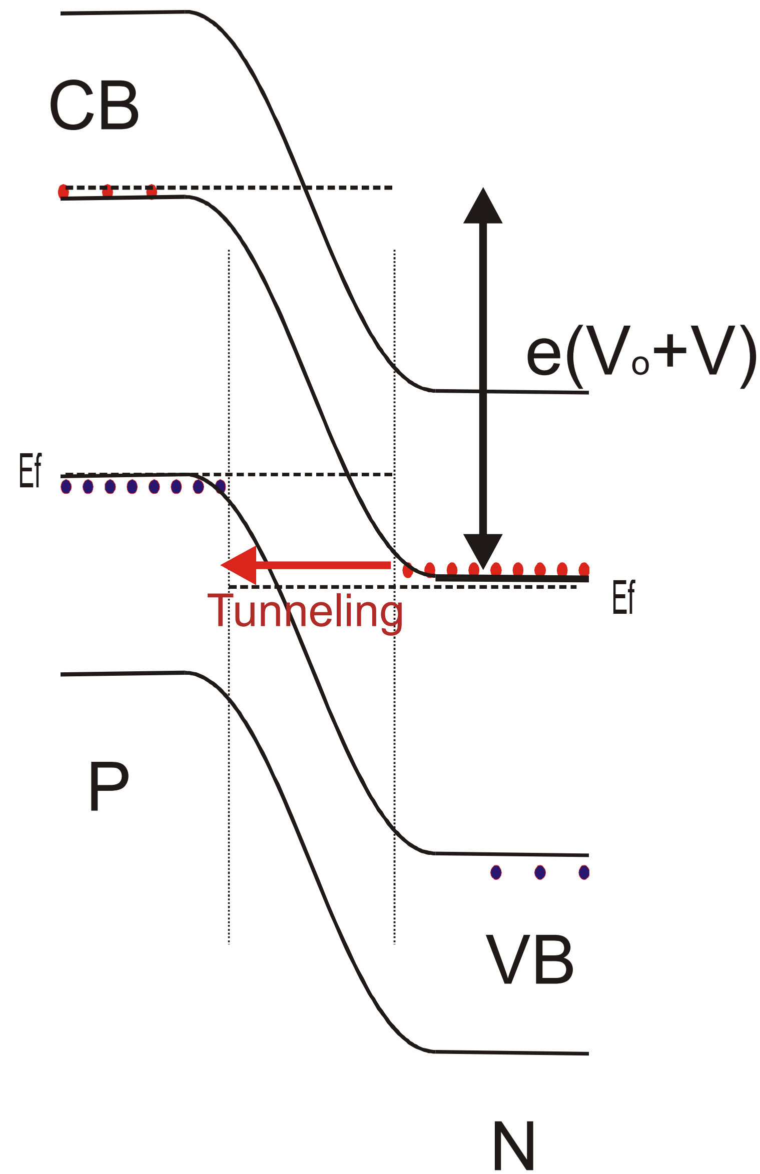
Practical examples of tunnelling:

A **Zener diode** is a type of diode that permits current to flow in the forward direction like a normal diode, but also in the reverse direction if the voltage is larger than the rated breakdown voltage known as the "Zener voltage".

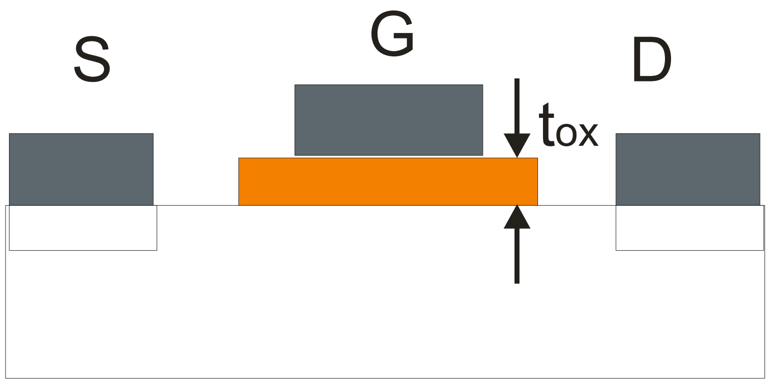
A conventional pn junction diode will not let significant current flow if reverse-biased below its reverse breakdown voltage. A **Zener diode** exhibits almost the same properties, except the device is especially designed so as to have a greatly reduced breakdown voltage, the so-called **Zener voltage**.

A Zener diode contains a heavily doped p-n junction allowing electrons to tunnel from the conduction band of the p-type material to the valence band of the n-type material. A reverse-biased Zener diode will exhibit a controlled breakdown and let the current flow to keep the voltage across the Zener diode at the Zener voltage. For example, a diode with a Zener breakdown voltage of 3.2 V will exhibit a voltage drop of 3.2 V if reverse biased..



MOSFET Gate Leakage

Oxide layer between the gate and channel is very thin for modern devices as miniaturisation proceeds, resulting in tunnelling through the oxide as the gate voltage increases. Gives a leakage current



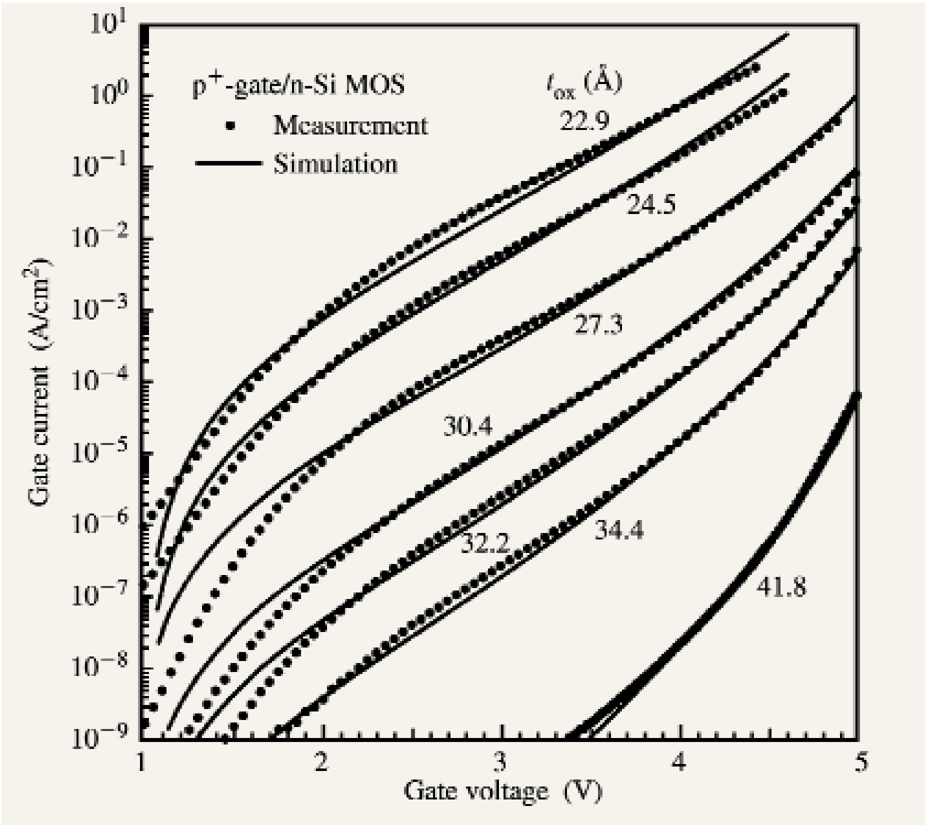


Figure 14

Measured and simulated I_G–V_G characteristics under accumulation conditions of p^+-gate/n-Si MOS devices with oxides ranging from 22.9 to 41.8 Å. The thickness is determined using the QM scheme.