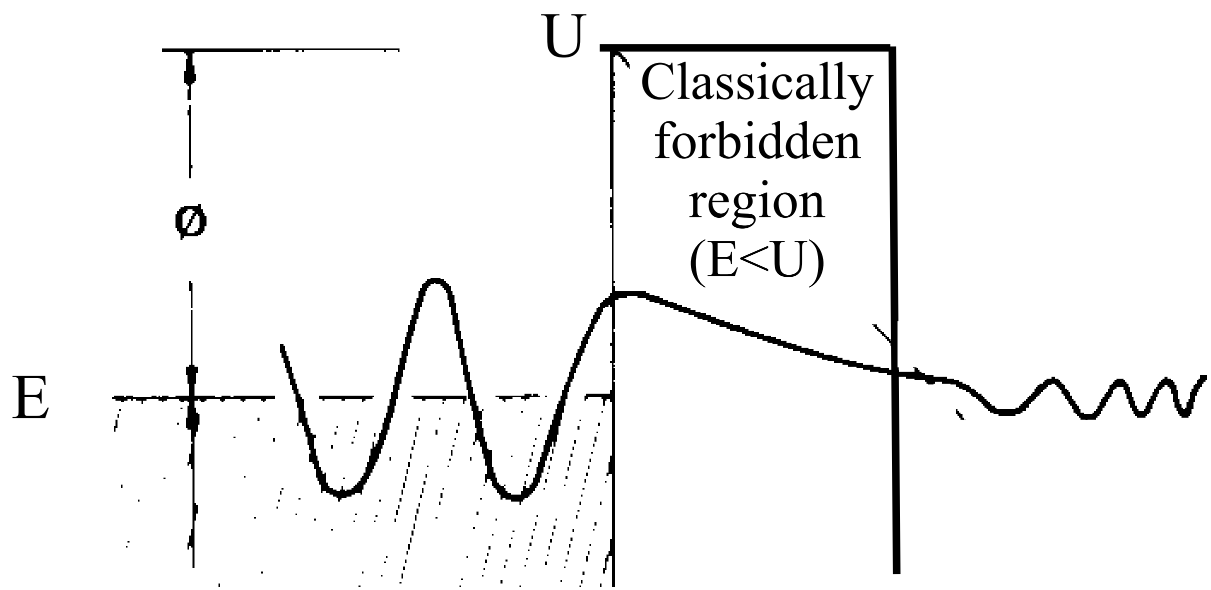
Quantum Mechanical Tunneling

- The quantum mechanical description of matter through wave-functions obeying the Schroedinger equation is consistent with the possibility of penetration through forbidden energy barriers
- The continuous nonzero nature of wave-functions, even in classically forbidden regions (negative kinetic energy), implies an ability to penetrate such forbidden regions and a probability of tunneling from one classically allowed region to another.

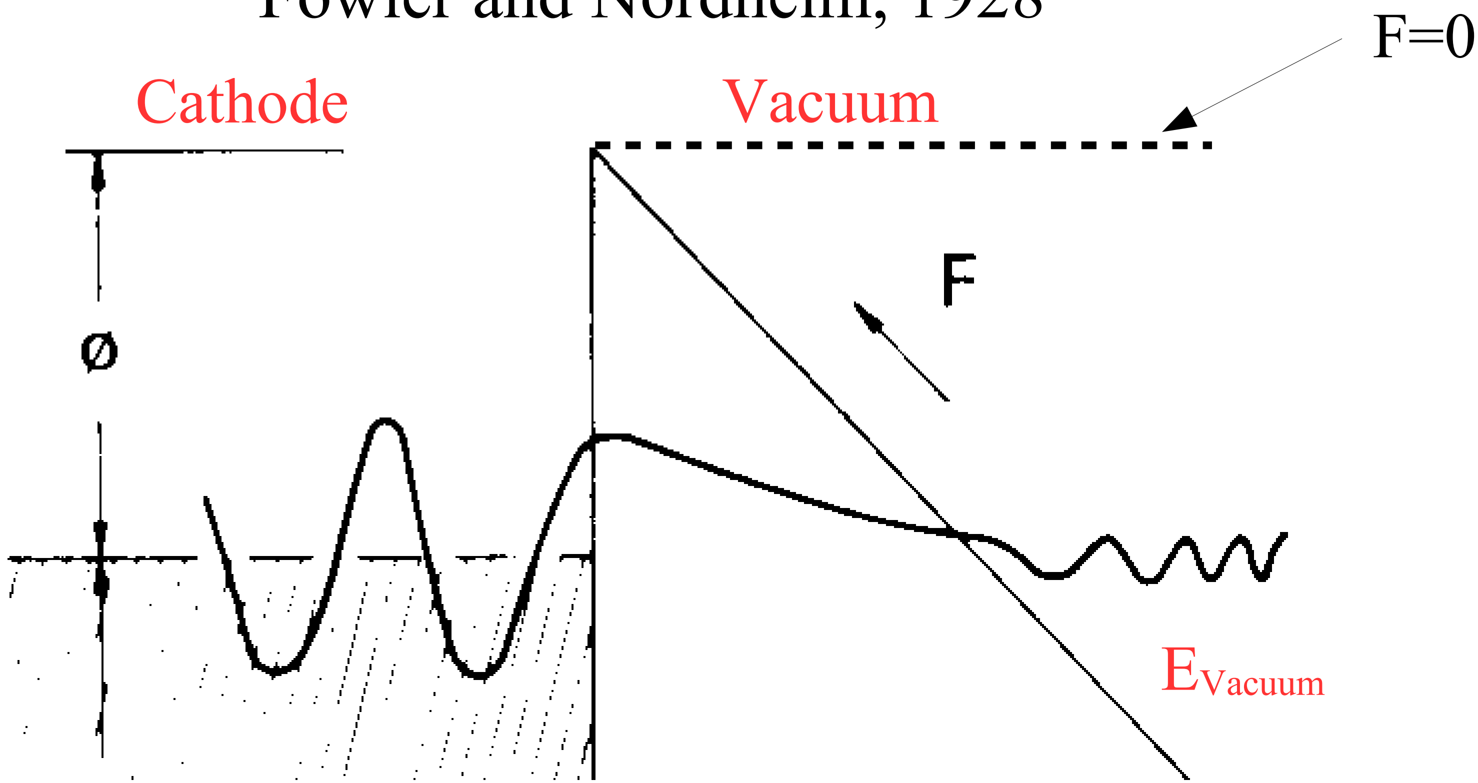


Quantum Mechanical Tunneling

- In 1928 Fowler and Nordheim explained, on the basis of electron tunneling, the main features of the phenomenon of electron emission from cold metals into vacuum, occurring due to high electric fields
- 1973 Nobel Prize for Physics awarded to Leo Esaki for the invention of the Tunnel Diode
- 1986 Nobel Prize for Physics awarded to G. Binning and H. Rohrer for the development of the Scanning Tunneling Microscope

Quantum Mechanical Tunneling
Field emission from cold cathodes

Fowler and Nordheim, 1928



$$J = A F^2 \exp\left(\frac{-4(2m)^{0.5}\phi^{1.5}}{3\hbar qF}\right)$$

F: electric field

$$\vec{F} = q\nabla E_{vacuum}$$

Picture from Esaki's Nobel Prize lecture

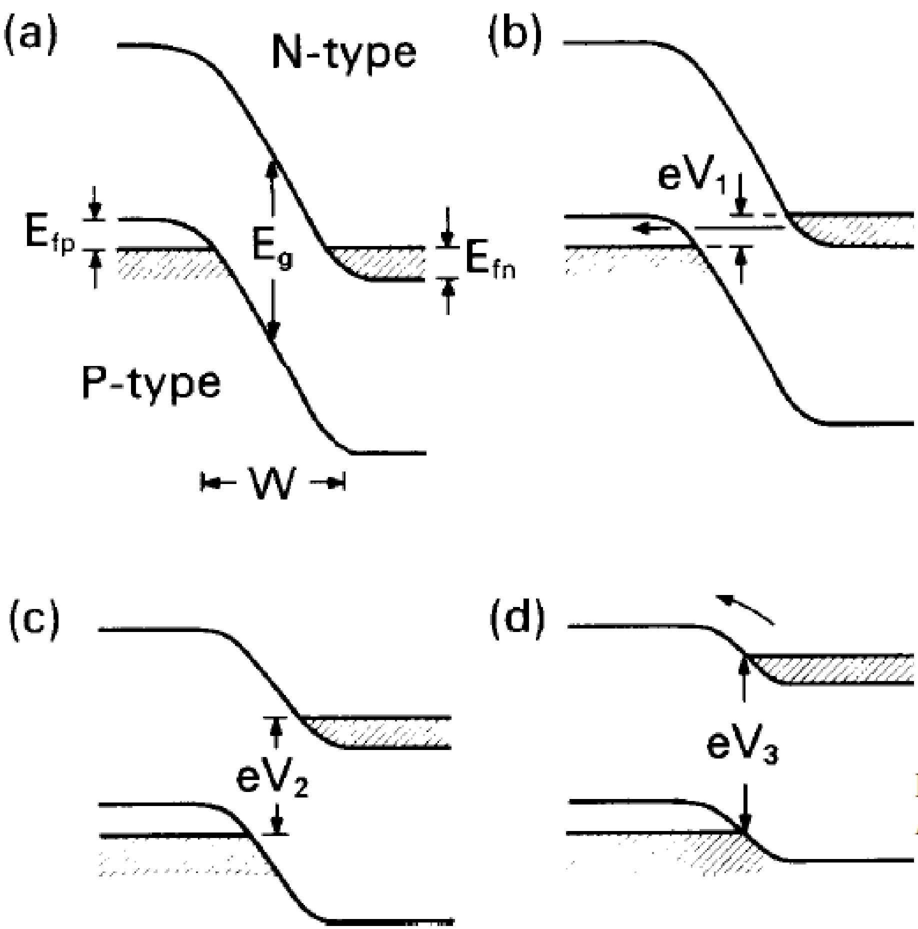
Quantum Mechanical Tunneling Esaki's tunnel diode

P-N junction with highly doped, degerate, N and P regions: E_F is positioned inside the conduction (valence) band in N (P) region.

For low positive bias (case b) an *energy window* exists, inside which electrons in conduction band of N-region can elastically tunnel into available valence-band states (holes) in P-region.

Larger positive bias (condition c) closes the *tunneling window*.

Further increasing the bias voltage leads to usual forward conduction of conventional diodes (region d).



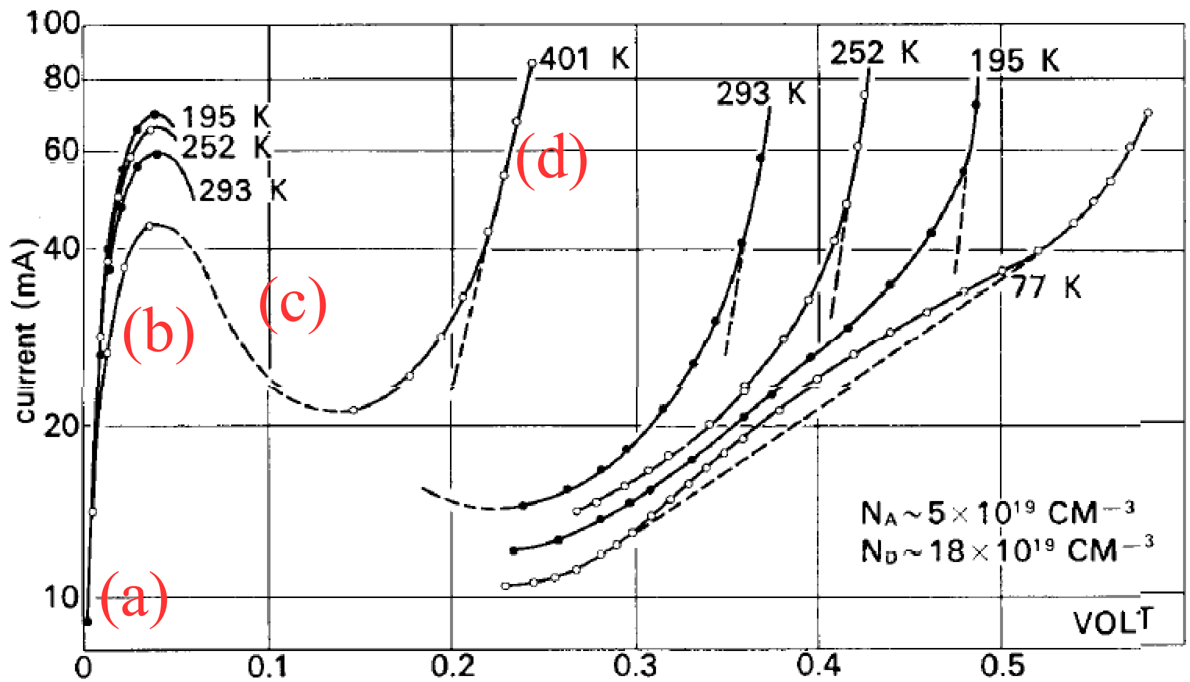
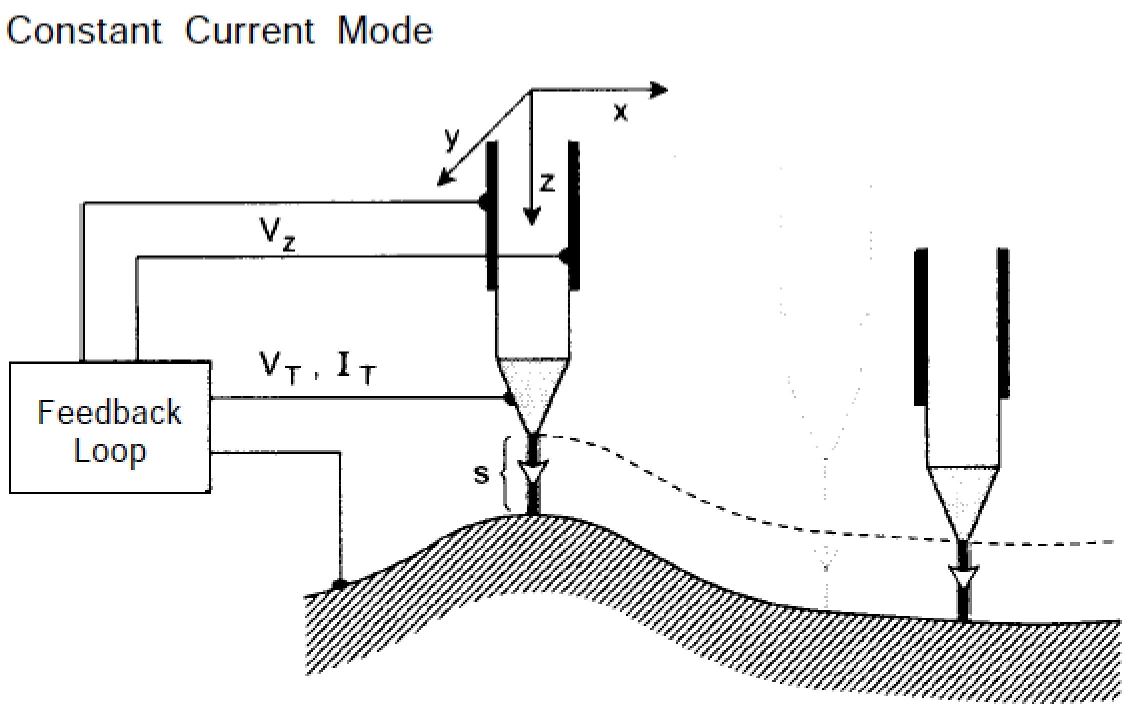


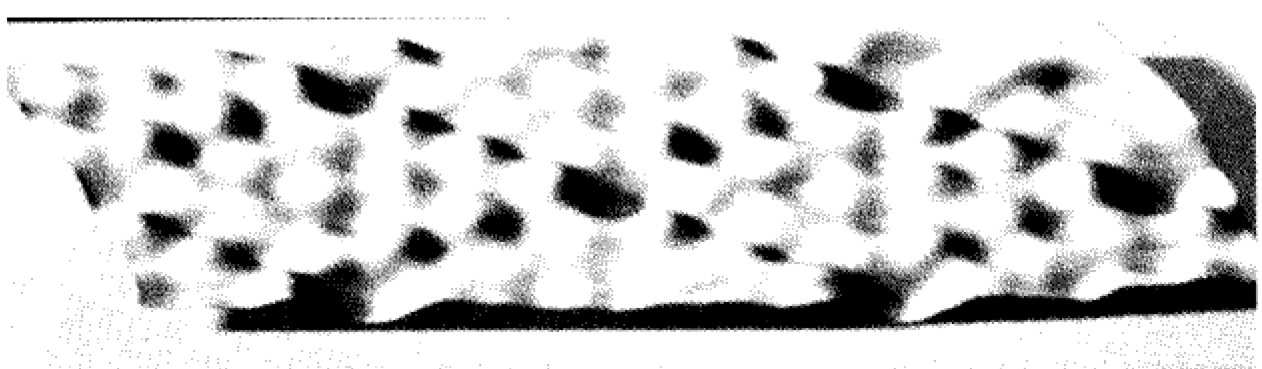
Fig. 4. Semilog plots of current-voltage characteristics in a tunnel diode, where $N_A \sim 5 \times 10^{19}$ cm^{-3} and $N_D \sim 1.8 \times 10^{19}$ cm^{-3}.

From Esaki's 1973 Physics Nobel Prize lecture

Quantum Mechanical Tunneling
Scanning tunneling microscopy



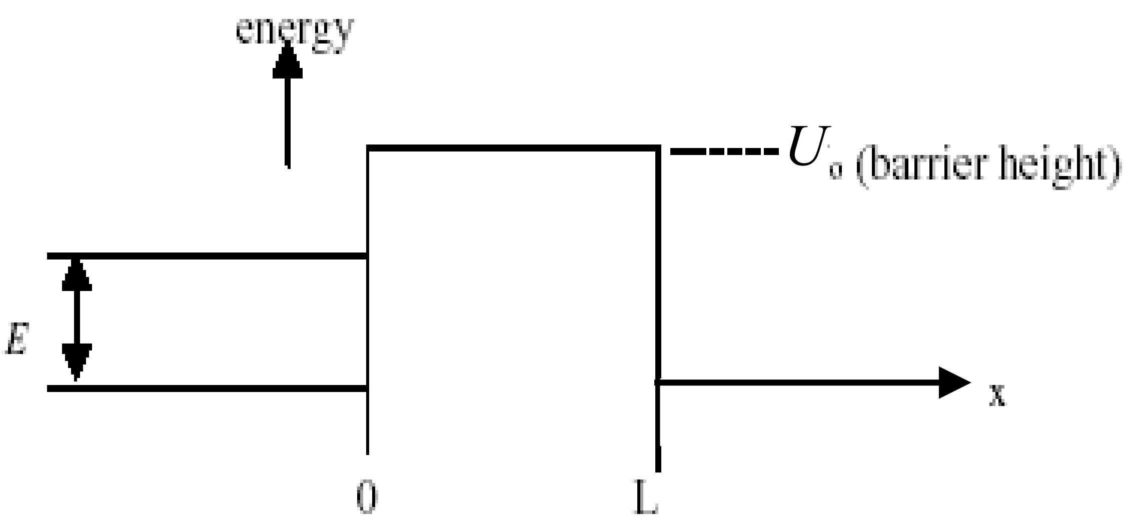
Constant current (I_T) mode: the tip is scanned across the surface at constant tunnel current, maintained at a pre-set value by continuously adjusting the vertical tip position with the feedback voltage V_Z. In the case of an electronically homogeneous surface, constant current essentially means constant s.

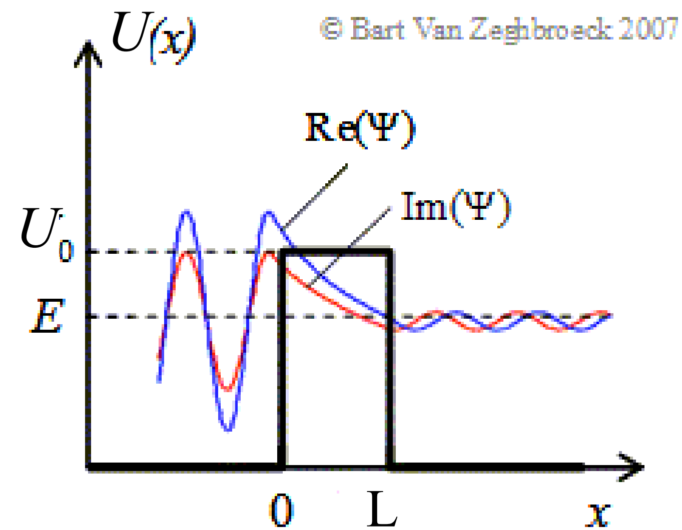


Si 111 surface

From Binning & Rohrer Nobel Prize lecture

Quantum Mechanical Tunneling





$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} E\psi = 0$$ outside barrier ($U = 0$)

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U_o)\psi = 0$$ inside barrier ($U = U_o$)

Quantum Mechanical Tunneling

Objective: given the barrier height U_0 and thickness L we want to find the probability for an electron to tunnel through the barrier

1) For x < 0, $U(x) = 0$ and the solution is same as for free electrons:

$$\psi(x) = A\exp(-jkx) + B\exp(jkx) \qquad k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Psi(x,t) = \psi(x)\cdot\phi(t) = A\exp[j(-kx+\omega t)] + B\exp[j(kx+\omega t)]$$

We can view this solution as sum of two travelling waves:

Incident $\quad \Psi_{inc}(x,t) = A\exp[j(-kx+\omega t)]$

Reflected $\quad \Psi_{refl}(x,t) = B\exp[j(kx+\omega t)]$

Quantum Mechanical Tunneling

2) <u>for 0 < x < L</u>, $\left(-\frac{\hbar^2}{2m}\right)\frac{d^2\psi}{dx^2} + U_o\psi = E\psi$

$$\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}(E - U_o)\psi =$$

Since $UE < V_o$ we rearrange the previous equation as

$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2}(U_o - E)\psi = 0 \quad \text{and define} \quad \alpha = \frac{\sqrt{2m(U_o - E)}}{\hbar}$$

so that

$$\frac{d^2\psi}{dx^2} - \alpha^2\psi = 0 \longrightarrow$$

exponential dumped solution

$$\psi(x) = C\exp(-\alpha x) + D\exp(\alpha x)$$

$$\Psi(x,t) = C\exp(-\alpha x + j\omega t) + D\exp[\alpha x + j\omega t]$$

Quantum Mechanical Tunneling

Assume forward transmission (single travelling wave past barrier)

3) For x > L,

$$\psi_{trans}(x) = F\exp(-jkx) \quad \Psi_{trans} = F\exp[j(-kx+\omega t)]$$

We now need to find A, B, C, D, F. We assume that $\psi(x)$ and $\frac{d\psi}{dx}$ are continuous at x = 0 and x = L.

By imposing the continuity of ψ and dψ/dx at x=0 (see next slide) and x= L we get a linear system in A,B,C,D,F.

$$A+B=C+D$$

$$-jkA+jkB=-\alpha C+\alpha D$$

$$C\exp(-\alpha L)+D\exp(\alpha L)=F\exp(-jkL)$$

$$-\alpha C\exp(-\alpha L)+\alpha D\exp(\alpha L)=-jkF\exp(-jkL)$$

Define a transmission coefficient $T=\left|\frac{\psi_{trans}(L)}{\psi_{inc}(0)}\right|^2=\left|\frac{F}{A}\right|^2=\left|\frac{4jk\alpha e^{jkL}}{(\alpha+jk)^2e^{\alpha L}-(\alpha-jk)^2e^{-\alpha L}}\right|^2$

and we find there is a non- zero probability of an electron penetrating barrier!

Quantum Mechanical Tunneling

Matching of solutions at x=0

Continuity of ψ(x) at x = 0

$$A\exp\left(-j\,k\,0^-\right)+B\exp\left(j\,k\,0^-\right)=C\exp\left(-\alpha\,0^+\right)+D\exp\left(\alpha\,0^+\right)$$

Continuity of ψ'(x) at x = 0

$$-j\,k\,A\exp\left(-j\,k\,0^-\right)+j\,k\,B\exp\left(j\,k\,0^-\right)=-\alpha\,C\exp\left(-\alpha\,0^+\right)+\alpha\,D\exp\left(\alpha\,0^+\right)$$

Similar matching conditions are set at x=L

QM-particles through barriers

Let's consider the solution inside the barrier:

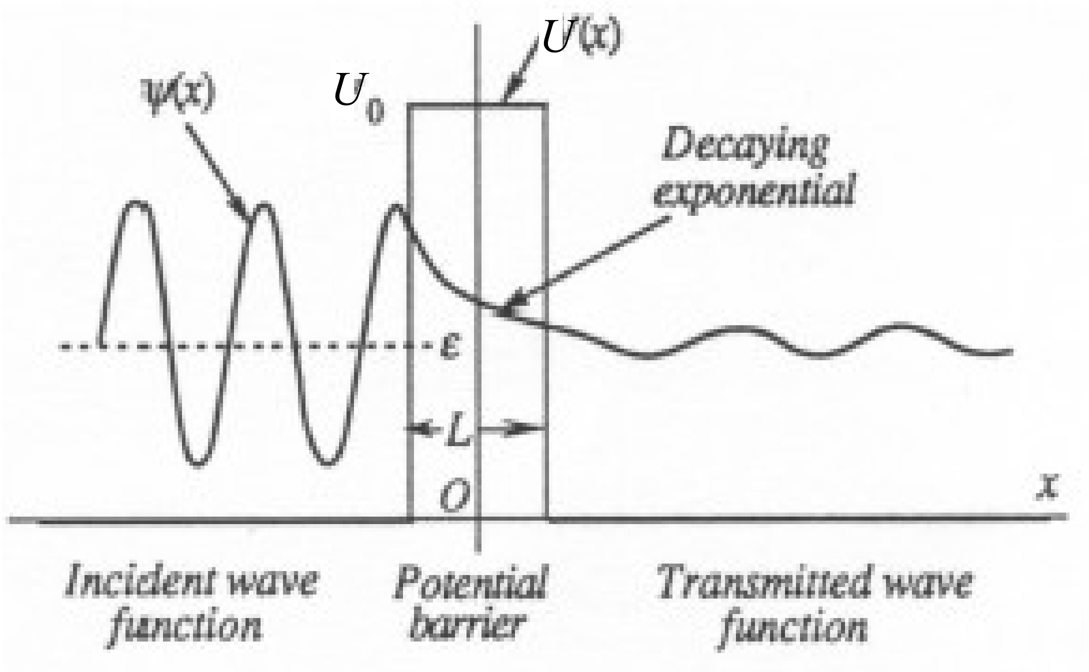
$$\psi(x) = C\exp(-\alpha x) + D\exp(\alpha x) \qquad \alpha = \frac{\sqrt{2m(U_0 - E)}}{\hbar}$$

Suppose that L is "large" compared to α^{-1} ($U_0 - E \gg \frac{\hbar^2}{2m}$, frequent case)

D exp(αx) diverges as x increases; the only acceptable solution requires: D=0

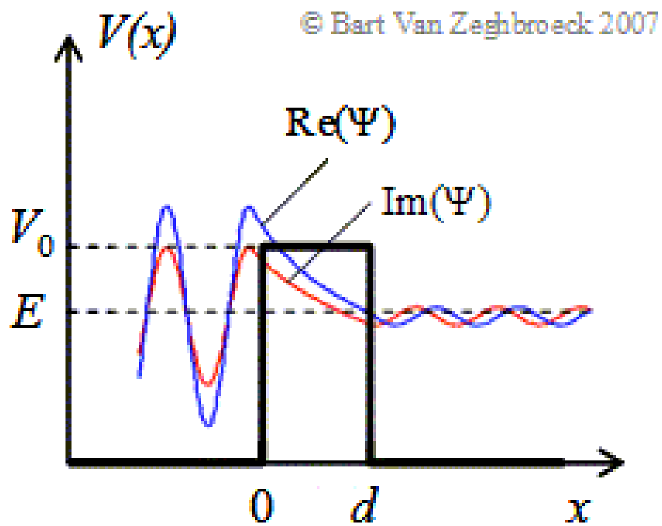
$$\psi(x) = C\exp(-\alpha x) \text{ (WKB approximation)}$$

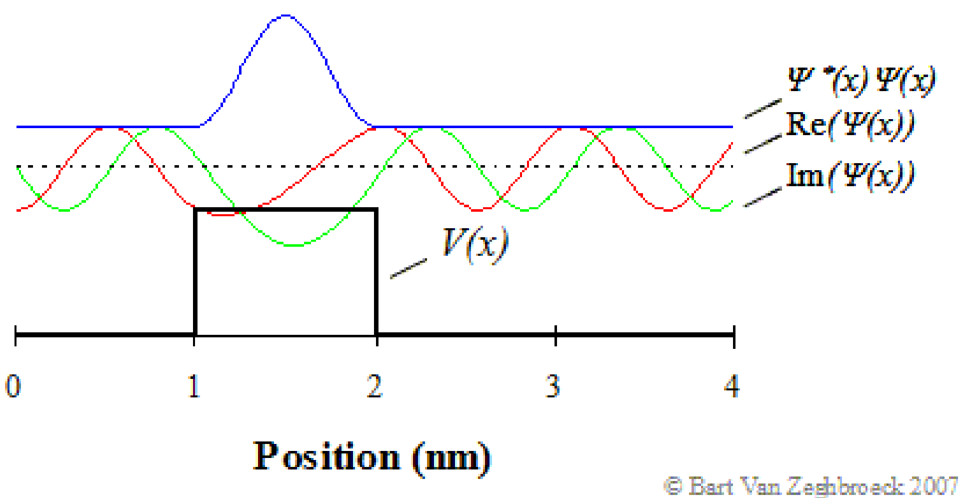
Probability of electrons penetrating the barrier: $T = \frac{|\psi(L)|^2}{|\psi(0)|^2} = \exp(-2\alpha L)$



Critical dependence of T on L and, through α, on the barrier height U_0 - E

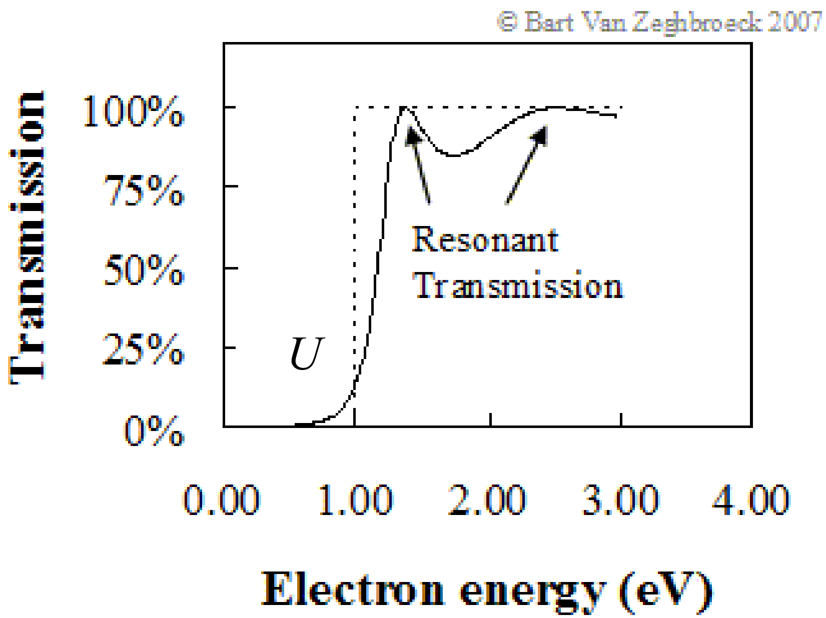
Tunneling through a 1nm thick, 1 eV high barrier



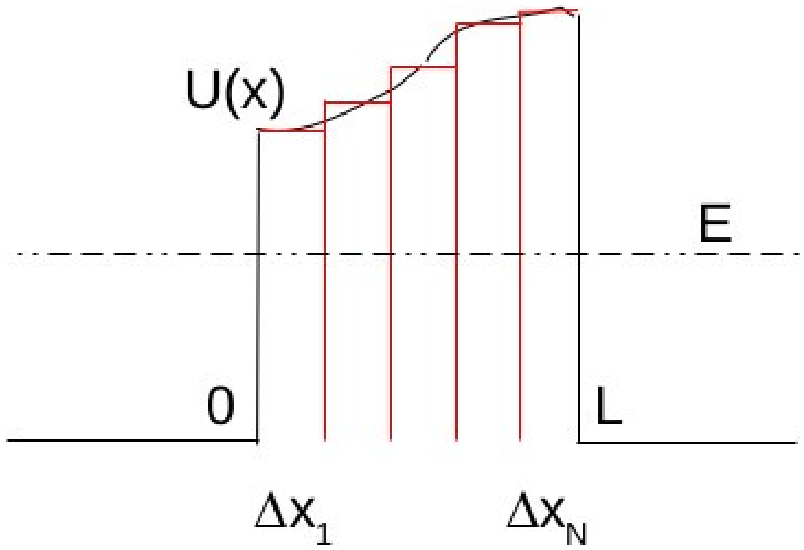


Transmission coef.

$$T = \frac{\left|\psi_{transm.}\right|^2}{\left|\psi_{incident}\right|^2}$$



Tunneling through a generic barrier



An energy barrier of arbitrary shape may be discretized into many sections of length dx_i, featuring approximately constant U_i values;

probability of tunneling through the i_{th} section: $T_i \approx e^{-2\alpha_i \delta x_i}$ with: $\alpha_i = \frac{\sqrt{2m(U_i - E)}}{\hbar}$

probability of tunneling through the entire barrier: $T \approx \prod_1^n e^{-2\alpha_i \delta x_i} = e^{-2\sum_1^n \alpha_i \delta x_i}$

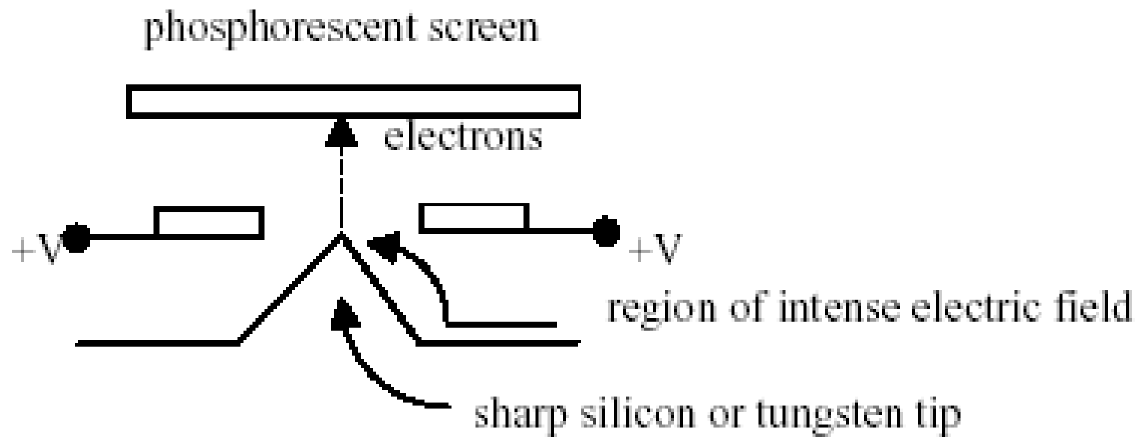
limit for infinitesimal discretization length dx:

$$T = \exp\left[-2\int_0^L \alpha(x)\,dx\right] = \exp\left[-2\frac{\sqrt{2m}}{\hbar}\int_0^L \sqrt{U(x) - E}\,dx\right]$$

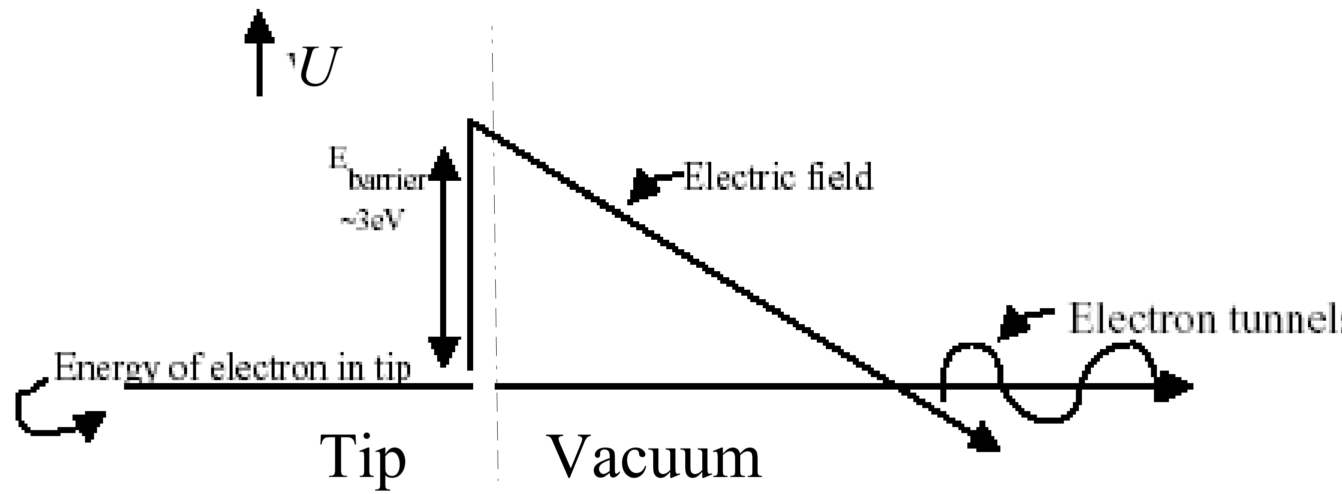
Field-emission from cold cathodes into vacuum

Practical Examples

a) Field emission displays:



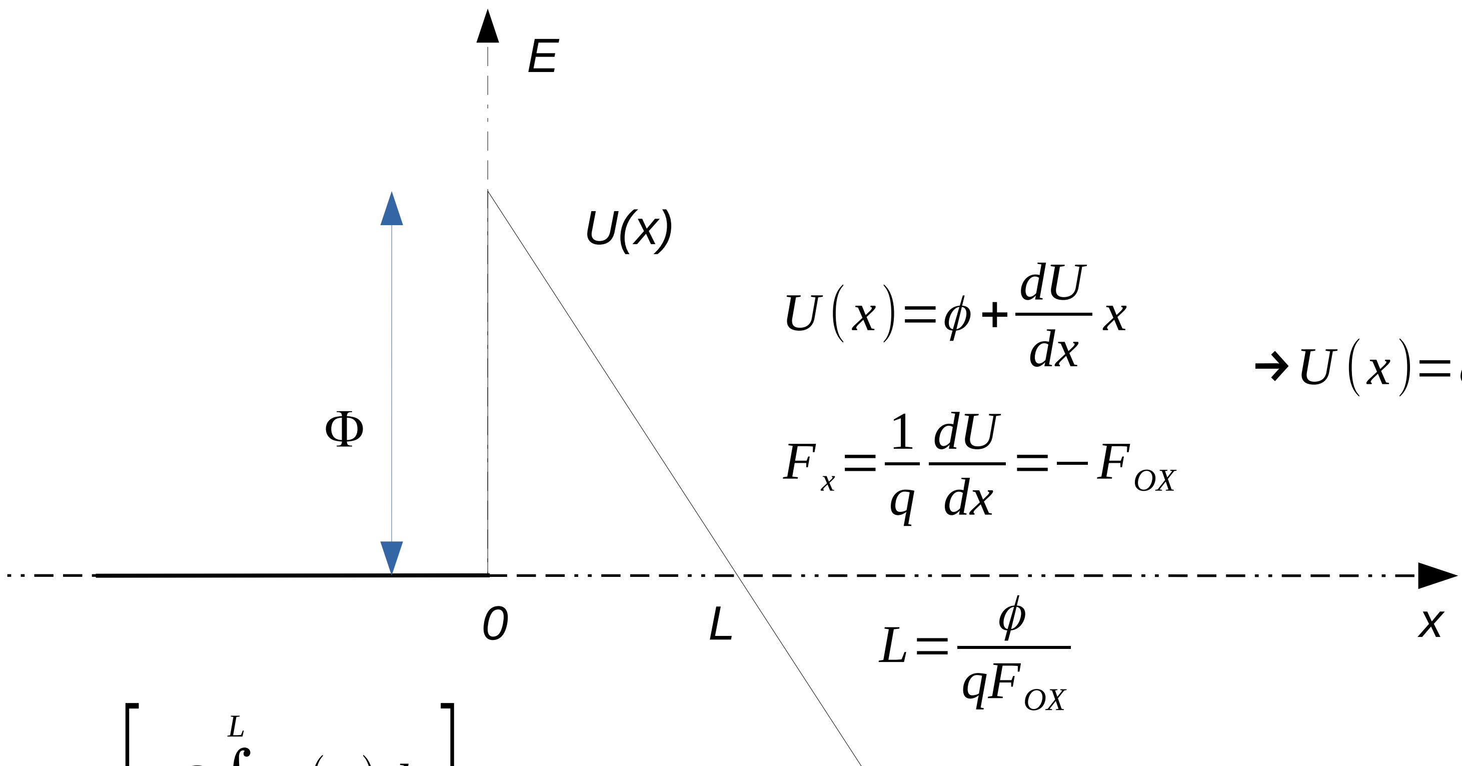
Electron energy diagram:



The electric field and potential energy are related by:

Electric field = $F_X = \frac{1}{q}\frac{dU}{x}$

Tunneling through triangular barrier (Fowler Nordheim)



$$U(x) = \phi + \frac{dU}{dx} x \quad \rightarrow U(x) = \phi - qF_{OX} x$$

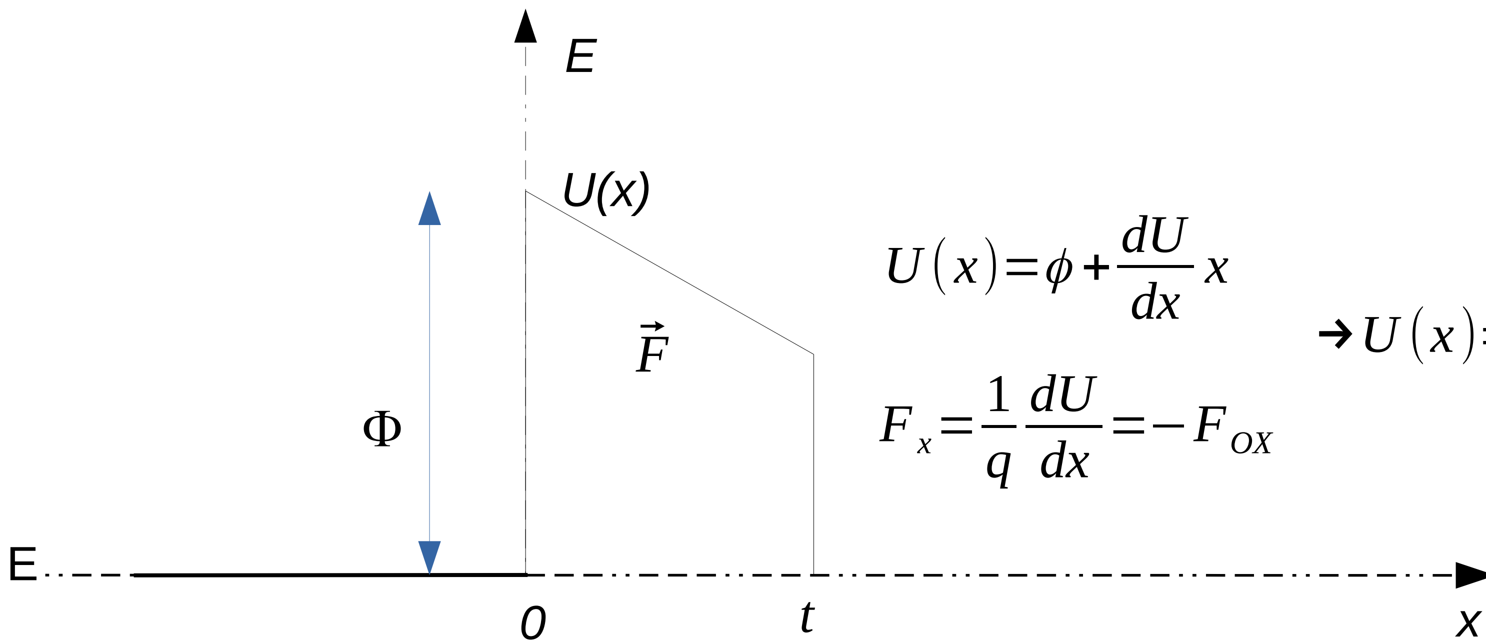
$$F_x = \frac{1}{q}\frac{dU}{dx} = -F_{OX}$$

$$L = \frac{\phi}{qF_{OX}}$$

$$T = \exp\left[-2\int_0^L \alpha(x)\,dx\right] \rightarrow T = \exp\left[\frac{-4(2m)^{0.5}\phi^{1.5}}{3\hbar q F_{OX}}\right]$$

$$\alpha(x) = \sqrt{\frac{2m}{\hbar^2}[U(x) - E_0]}$$

Tunneling through trapezoidal barrier (Direct Tunneling)



$$U(x)=\phi+\frac{dU}{dx}x$$

$$F_x=\frac{1}{q}\frac{dU}{dx}=-F_{OX}$$

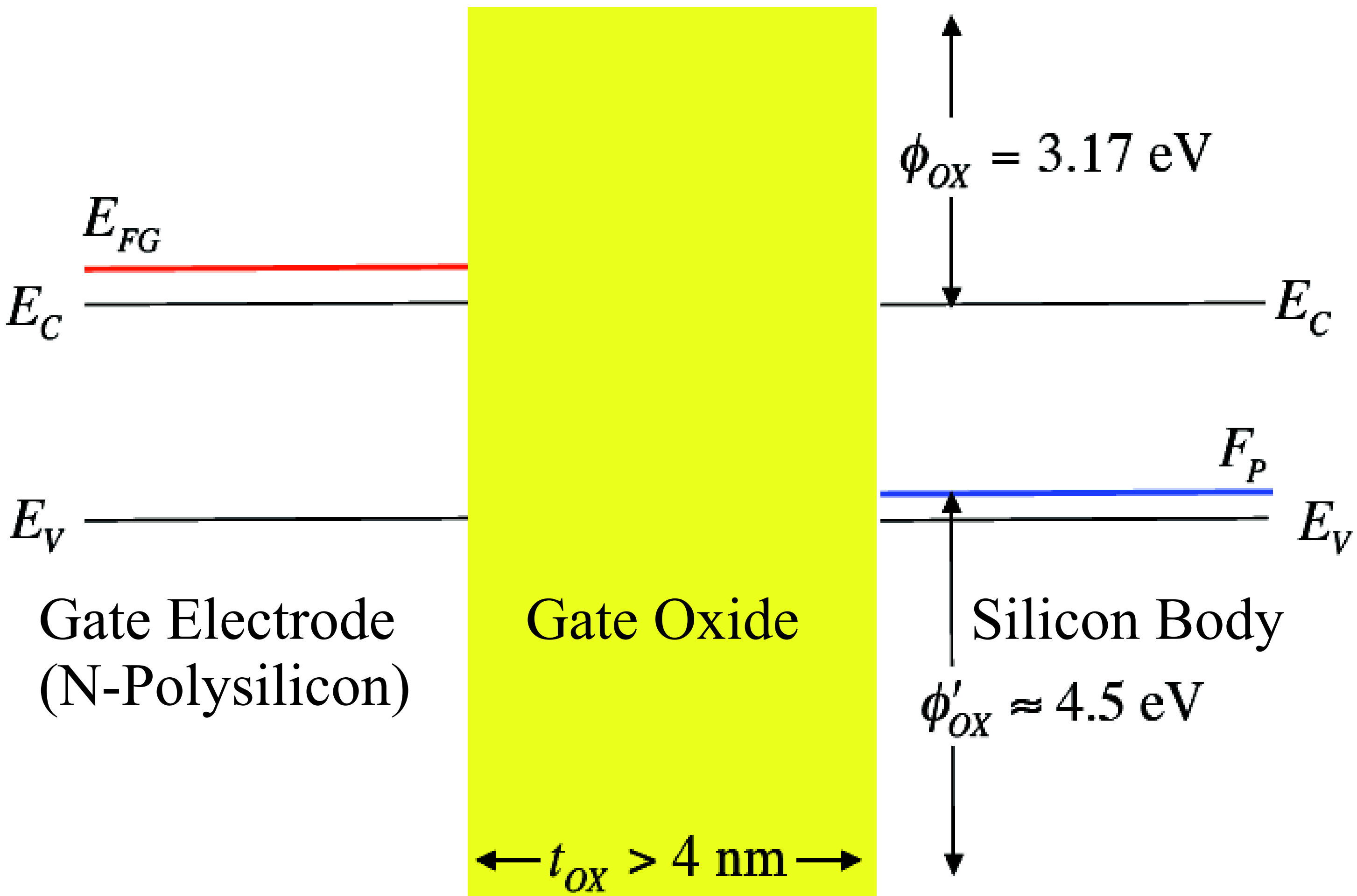
$$\rightarrow U(x)=\phi-qF_{OX}x$$

$$T=\exp\left[-2\int_0^t \alpha(x)\,dx\right]$$

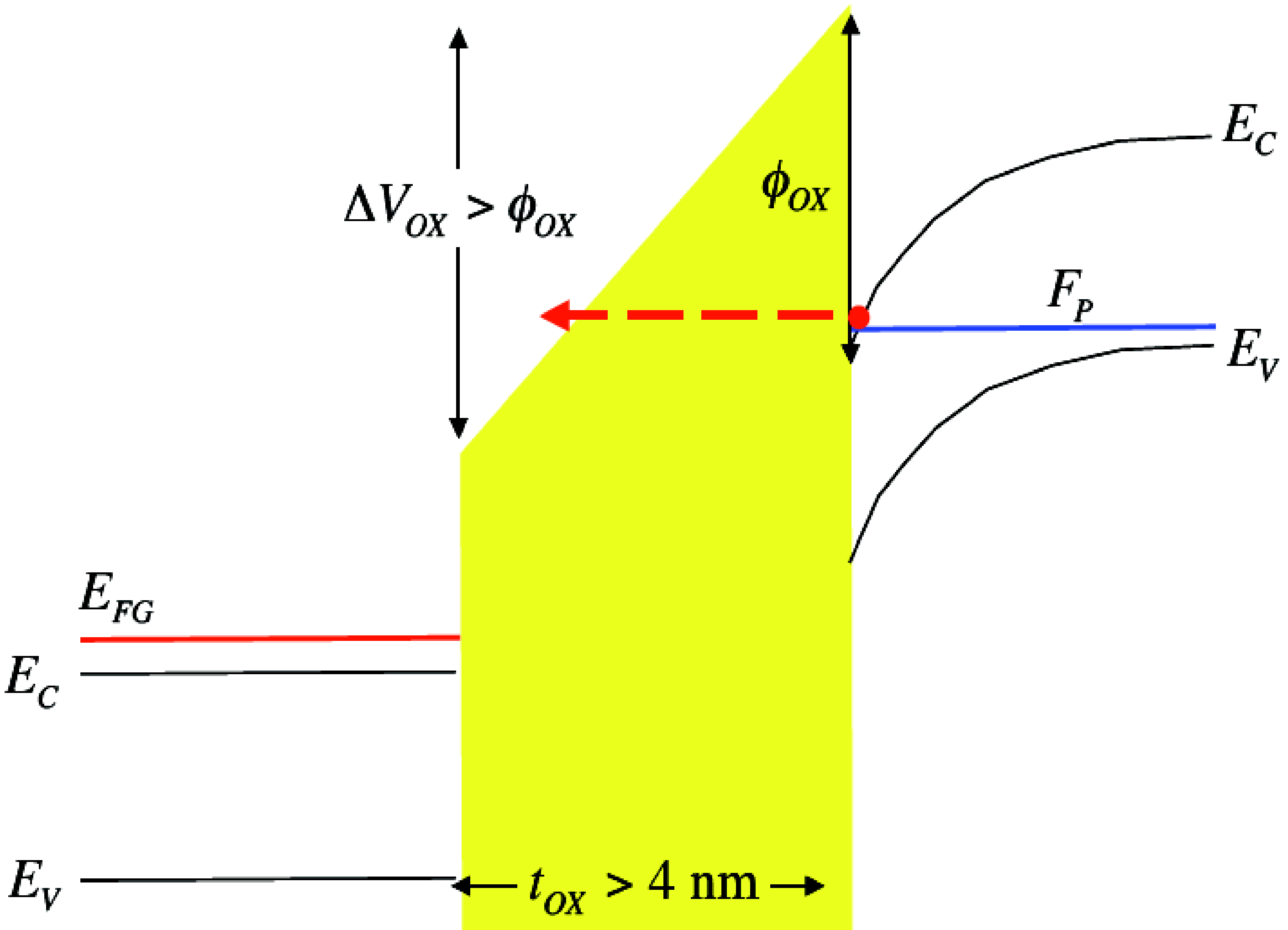
$$\alpha(x)=\sqrt{\frac{2m}{\hbar^2}[U(x)-E]}$$

if $\phi \gg qF_{OX}t$ $\longrightarrow$ $T\simeq\exp\left[\frac{-2(2m\phi)^{0.5}t}{\hbar}\right]$

gate leakage



Fowler-Nordheim tunneling



Fowler-Nordheim tunneling (ii)

3

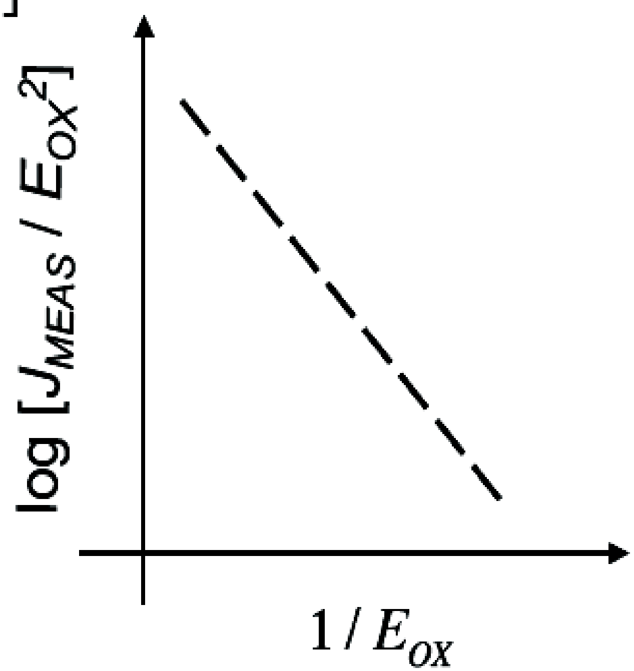
$$J_{FN} = \frac{q^3 E_{OX}^2}{16\pi^2 \hbar \phi_{OX}} \exp\left[-\frac{4\sqrt{2m^* \phi_{OX}^{3/2}}}{3\hbar q E_{OX}}\right]$$ eqn. (2.209) Taur and Ning

E_{OX}: electric field in the oxide

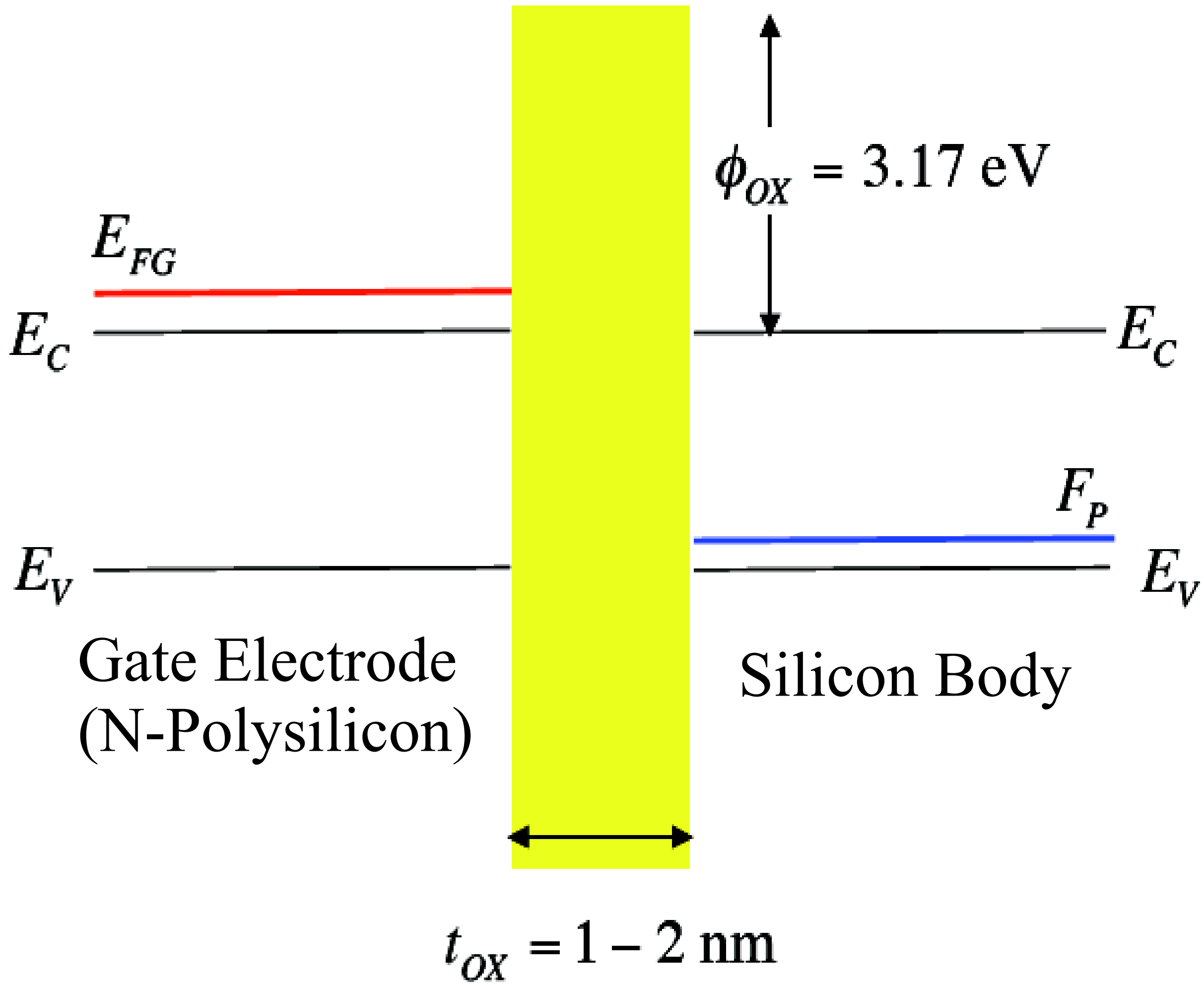
$$J_{FN} / C_1 E_{OX}^2 = \exp\left[-\frac{C_2}{E_{OX}}\right]$$

$$E_{OX} = 8 \text{ MV/cm}$$

$$J_{FN} = 5 \times 10^{-7} \text{ A/cm}^2$$

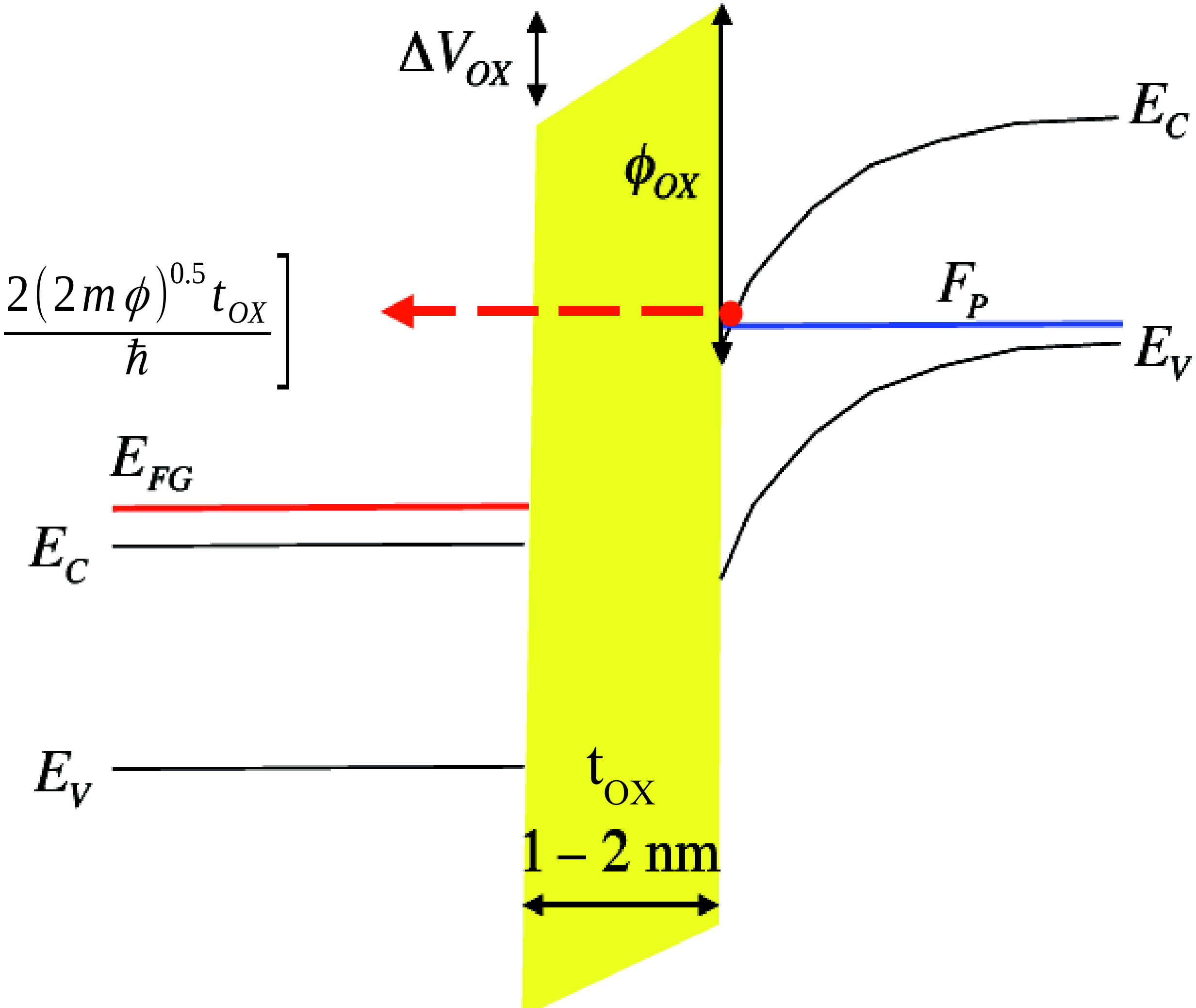


gate leakage (thin oxides)

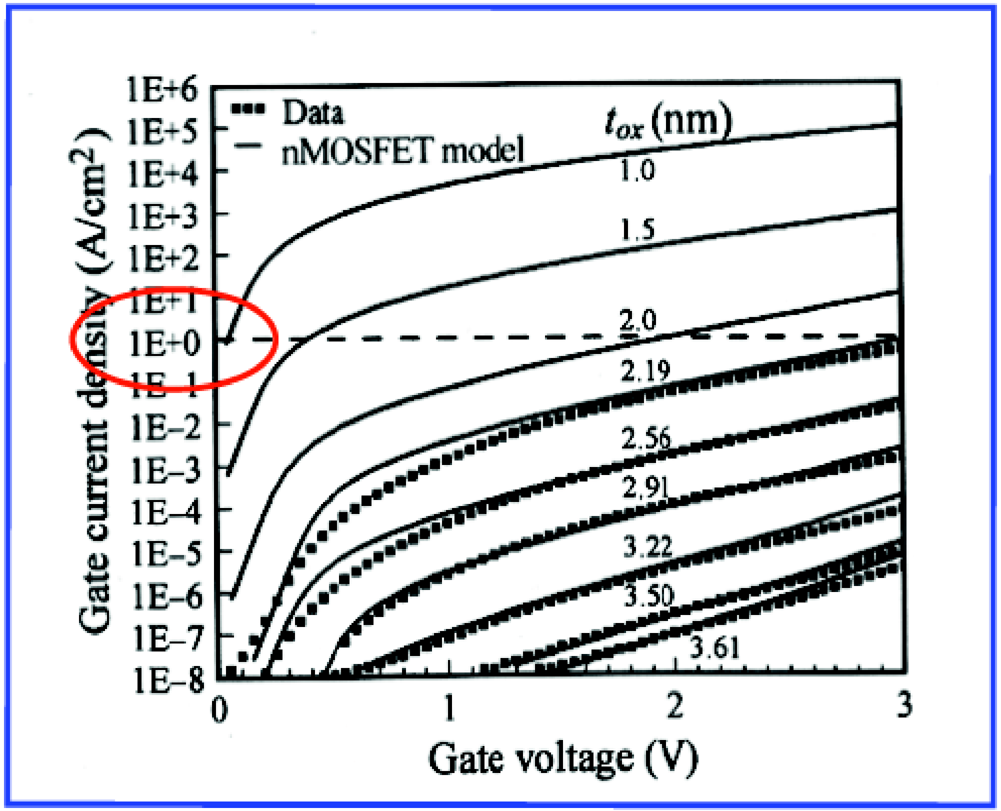


direct tunneling

$$T \simeq \exp\left[-\frac{2(2m\phi)^{0.5}t_{OX}}{\hbar}\right]$$

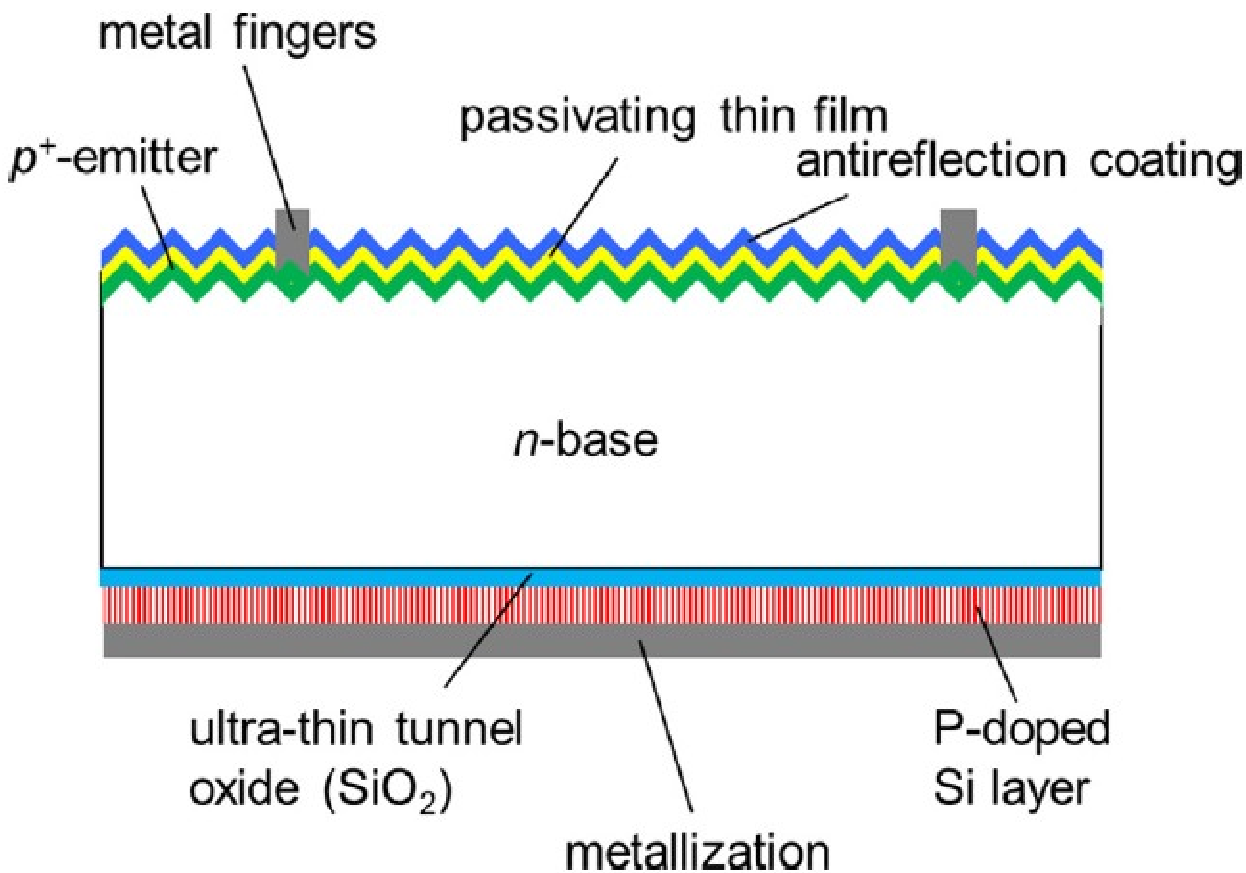


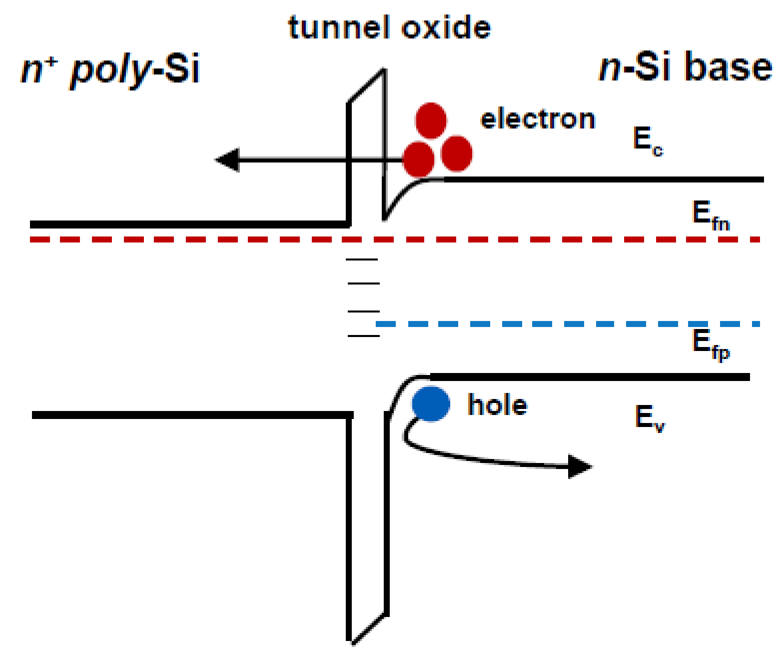
direct tunneling in practice



Lo, Buchanan, and Taur, "Modeling and characterization of quantization, polysilicon depletion, and direct tunneling effects in MOSFETs with ultrathin oxides," *IBM J. Res. Develop.*, **43**, pp. 327-337, 1999.

Exploitation of direct tunneling in advanced solar cells





Passivated tunneling back contact
Avoids charge recombination at the back cell contact
Conversion efficiency up to 25.1% demonstrated (Lab.)