Notes for
ECE-606: Spring 2013

L3: Quantum Mechanics

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1/14/13

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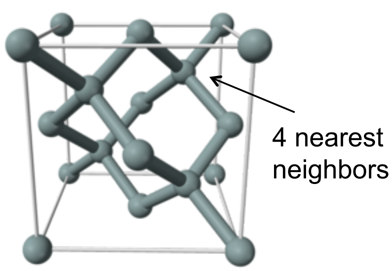
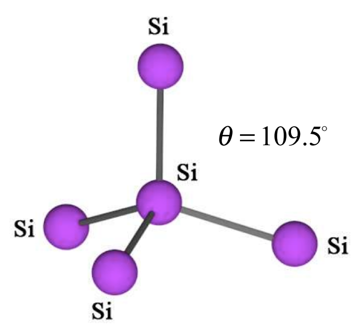
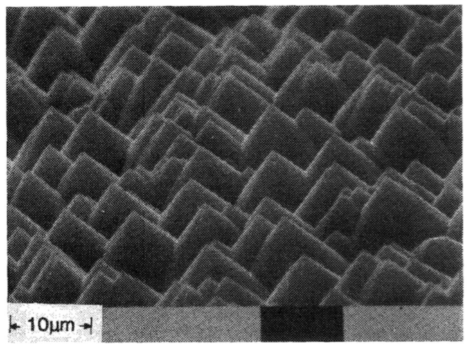
tetrahedral bonding in the diamond lattice





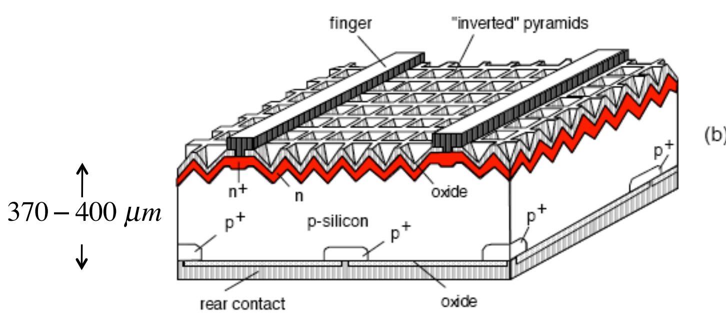
J. S. Bhosale, Ph.D. defense, 1/11/13

Anisotropic etching of Si



P. Campbell, P. M.A. Green, "Light trapping properties of pyramidally textured surfaces," *J. Appl. Phys*. **62**, 243-249 (1987).

Anisotropic etching of Si



24.5% at 1 sun

Martin Green Group UNSW – Zhao, et al, 1998

motivation for quantum mechanics

1) Black body radiation (Planck)

$$E = hf = \hbar\omega$$

2) Photoelectric effect (Einstein)

$$E = hf = \hbar\omega$$

3) Atomic spectra (Bohr)

4) Wave-particle duality (de Broglie)

$$p = \hbar k = h/\lambda$$

Schroedinger wave equation

$$KE + PE = E$$

$$\Psi(x,t) = e^{i(kx-\omega t)}$$

$$KE = \frac{p^2}{2m_0}$$

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t) = \hbar k\Psi(x,t)$$

$$\hat{p}\Psi(x,t) = \hbar k\Psi(x,t)$$

$$\hat{p} \equiv \frac{\hbar}{i}\frac{\partial}{\partial x}$$

$$\hat{p}\left[\hat{p}\Psi(x,t)\right] = (\hbar k)^2\Psi(x,t)$$

$$-\hbar^2\frac{\partial^2}{\partial x^2}\Psi(x,t) = (\hbar k)^2\Psi(x,t)$$

$$\hat{p}^2\Psi(x,t) = -\hbar^2\frac{\partial^2}{\partial x^2}\Psi(x,t)$$

$$\frac{\hat{p}^2}{2m_0}\Psi(x,t) = \frac{-\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2}\Psi(x,t)$$

$$= \frac{\hbar^2k^2}{2m_0}\Psi(x,t)$$

$$= KE\Psi(x,t)$$

Schroedinger wave equation

$$(KE)\Psi(x,t)+PE\,\Psi(x,t)=E\Psi(x,t)$$

$$\Psi(x,t)=e^{i(kx-\omega t)}$$

$$PE=U(x)$$

$$\frac{-\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2}\Psi(x,t)+U(x,t)\Psi(x,t)=E\Psi(x,t)$$

$$-\frac{\hbar}{i}\frac{\partial}{\partial t}\Psi(x,t)=\hbar\omega\,\Psi(x,t)$$

$$\hat{E}=-\frac{\hbar}{i}\frac{\partial}{\partial t}$$

$$\hat{E}\Psi(x,t)=\hbar\omega\,\Psi(x,t)$$

$$\frac{-\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2}\Psi(x,t)+U(x,t)\Psi(x,t)=-\frac{\hbar}{i}\frac{\partial\Psi(x,t)}{\partial t}$$

Time-independent Schroedinger wave equation

$$\frac{-\hbar^2}{2m_0}\frac{\partial^2}{\partial x^2}\Psi(x,t)+U(x,t)\Psi(x,t)=-\frac{\hbar}{i}\frac{\partial\Psi(x,t)}{\partial t}$$

$\Psi(x,t)=\psi(x)\phi(t)$ "separation of variables"

$$\frac{-\hbar^2}{2m_0}\frac{\partial^2\psi(x)}{\partial x^2}\phi(t)+U(x,t)\psi(x)\phi(t)=-\frac{\hbar}{i}\frac{\partial\phi(t)}{\partial t}\psi(x)$$

$$\frac{-\hbar^2}{2m_0}\frac{\partial^2\psi(x)}{\partial x^2}\frac{1}{\psi(x)}+U(x)=-\frac{\hbar}{i}\frac{\partial\phi(t)}{\partial t}\frac{1}{\phi(t)}$$

Time independent Schroedinger wave equation

$$\frac{-\hbar^2}{2m_0}\frac{\partial^2\psi(x)}{\partial x^2}\frac{1}{\psi(x)}+U(x)=c \qquad -\frac{\hbar}{i}\frac{\partial\phi(t)}{\partial t}\frac{1}{\phi(t)}=c$$

$$\frac{-\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2}+U(x)\psi(x)=E\psi(x)$$

$$\Psi(x,t)=\psi(x)\phi(t)=\psi(x)e^{-i\omega t}$$

$$\omega=\frac{E}{\hbar}$$

$$-\frac{\hbar}{i}\frac{\partial\phi(t)}{\partial t}=c\phi(t)$$

$$\phi(t)=e^{-i\omega t}$$

$$-\frac{\hbar}{i}\frac{\partial\phi(t)}{\partial t}=\hbar\omega\phi(t)=c\phi(t)$$

$$c=\hbar\omega=E$$

Time independent Schroedinger wave equation

$$\frac{\partial^2\psi(x)}{\partial x^2}+\frac{2m_0}{\hbar}\left[E-U(x)\right]\psi(x)=0$$

$E>U(x)$

$$\frac{-\hbar^2}{2m_0}\frac{d^2\psi(x)}{dx^2}\frac{1}{\psi(x)}+U(x)$$

$$k^2=\frac{2m_0}{\hbar}\left[E-U(x)\right]$$

$$\psi(x)=Ae^{\pm ikx}$$

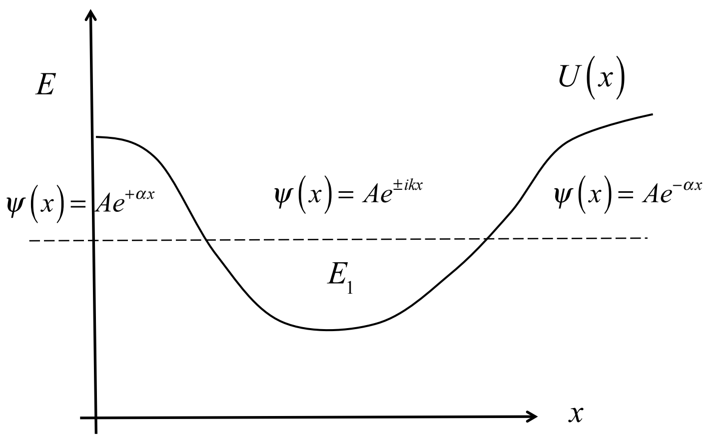
$E<U(x)$

$$\frac{\partial^2\psi(x)}{\partial x^2}-\alpha^2\psi(x)=0$$

$$\alpha^2=\frac{2m_0}{\hbar}\left[U(x)-E\right]$$

$$\psi(x)=Ae^{\pm\alpha x}$$

solutions of the SE



quantum effects

1) Plane waves
2) Quantum confinement
3) Quantum reflection and tunneling
4) Plane waves **and** quantum confinement

Plane waves

$$\frac{d^2\psi(x)}{dx^2} + \frac{2m_0}{\hbar}\left[E - U_0\right]\psi(x) = 0$$

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi(x) = 0$$

$$\psi(x) = Ae^{\pm ikx}$$

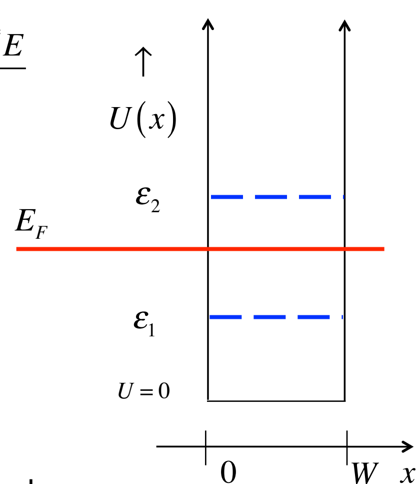
$$\psi(x) = \frac{1}{\sqrt{L}}e^{ikx}$$ (normalized in 1D)

particle in a box

$$\frac{d^2\psi(x)}{dx^2} + k^2\psi = 0 \qquad k^2 = \frac{2m^*E}{\hbar^2}$$

$$\psi(x) = \sin k_n x$$

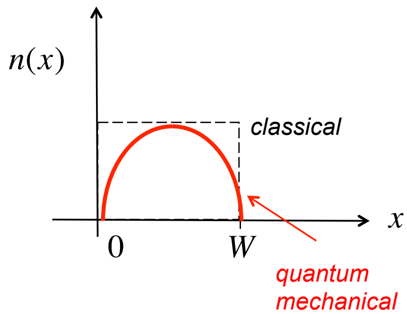
$$\varepsilon_n = \frac{\hbar^2 k_n^2}{2m^*} = \frac{\hbar^2 n^2 \pi^2}{2m^* W^2}$$



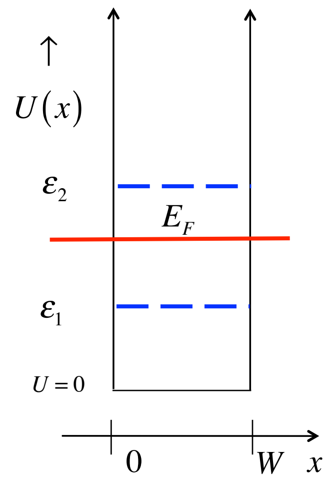
light mass
narrow width

ε high subband energy

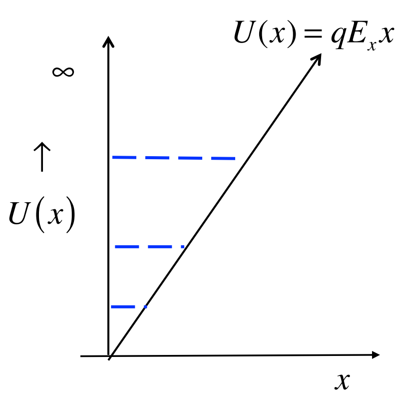
carrier densities

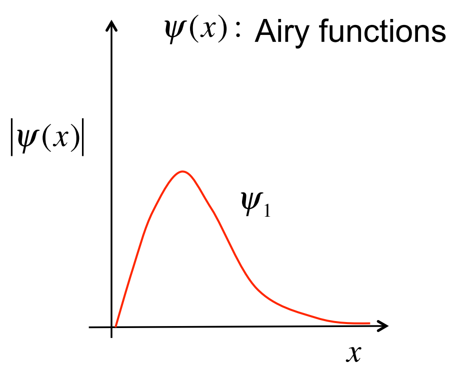


$$n(x) \propto \psi^*(x)\psi(x)$$



triangular quantum well





$$\varepsilon_i = \left[\frac{3hqE_x}{4\sqrt{2m^*}}(i+3/4)\right]^{2/3} \quad i = 1,2,3,\ldots \quad \langle x \rangle = \frac{2E_i}{3qE}$$

quantum effects

1) Plane waves

2) Quantum confinement

3) Quantum reflection and tunneling

4) Plane waves **and** quantum confinement