3.024

“Electronic, Optical, and Magnetic Properties of Materials”

3.024
The Final

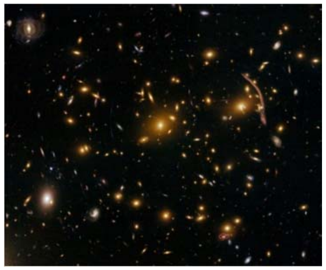
- **The final exam will be focused on the second half of the class, but knowledge of basic quantum concepts and potentials is a must.**
- **There will be no complicated equations, so you won’t need an equation sheet. Concepts come first.**
- **Bring your brain, pens, pencils and a calculator (strongly recommended).**

3.024 Topics Discussed

- **Hamiltonian mechanics with application to normal vibrations in crystals**
  Phonons: dispersion relations, normal modes.
- **Introduction to Quantum Mechanics: Schrodinger's Equation.**
  Applications to quantum dots, tunneling devices.
- **Localized vs. delocalized states: from a free electron to an atom.**
- **Electronic states in crystals: DOS, bandgaps, interpretation of band diagrams.**
- **Fermions, symmetrization and Pauli's exclusion principle:**
  Electrons in bands and the classification of solids.
- **"Free electron gas" description of carriers**
- **The chemical potential: Fermi level, statistics of electron distribution.**
- **Electronic structure of semiconductors: intrinsic and extrinsic.**
- **Semiconductor devices: p-n junctions under illumination and applied voltage.**
- **Maxwell's equations: electromagnetic waves in materials.**
- **Indices of refraction: reflection and transmission.**
- **Periodic optical materials: photonic bands and bandgaps.**
- **Magnetization in materials: para-, ferro-, anti-ferro and ferrimagnets.**
- **Magnetic domains.**

Quantum Mechanical Potentials

Particle in Free space



Gravitational lensing in the Abel 370 galaxy cluster. (Photo courtesy of NASA, ESA, the Hubble SM4 ERO Team and ST-ECF http://www.spacetelescope.org/images/heic0910b/.)

Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Energy eigenvalues:

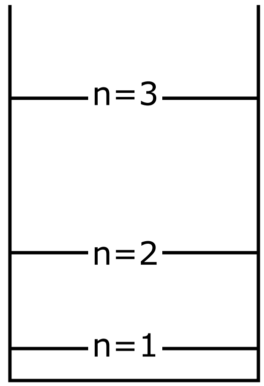
$$E_n = \frac{\hbar^2 k^2}{2m}$$

Energy eigenfunctions:

$$u_k(x) = e^{\pm ikx}$$

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

Particle in 1D box



Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$$V(x) = \begin{cases} 0, & 0 \le x \le d \\ \infty, & x > d \;\&\; x < 0 \end{cases}$$

Energy eigenvalues:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2md^2}$$

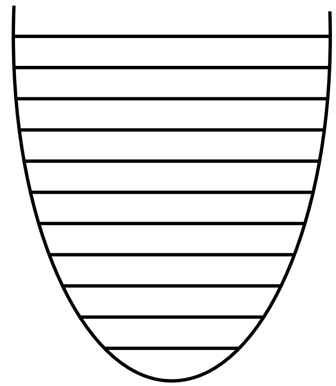
$$\Delta E_n = E_{n+1} - E_n = \frac{\hbar^2 \pi^2}{2md^2}(2n+1)$$

Energy eigenfunctions:

$$u_n(x) = A_n \sin\frac{n\pi x}{d}$$

$$A_n = \sqrt{\frac{2}{d}}$$

1D SHO



Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2 x^2$$

Energy eigenvalues:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

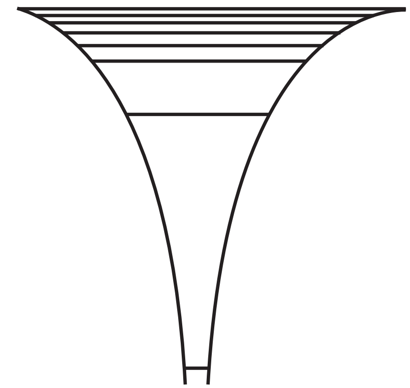
$$\Delta E_n = E_{n+1} - E_n = \hbar\omega$$

Energy eigenfunctions:

$$u_n(x) = e^{-\frac{m\omega}{2\hbar}x^2} h_n(x)$$

$$h_n(x) - Hermite\ polynomial$$

Hydrogen atom



Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m_r}\nabla^2 - \frac{e^2}{r}$$

Energy eigenvalues:

$$E_n = -\frac{E_I}{n^2}$$

$$\Delta E_n = E_{n+1} - E_n = \frac{(2n+1)E_I}{n^2(n+1)^2}$$

Energy eigenfunctions:

$$u_n(x) = R_{nl}(r) Y_l^m(\theta, \varphi)$$

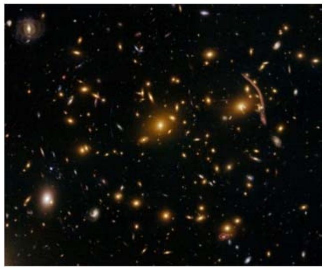
$$0 \le l \le n-1$$

$$-l+1 \le m \le l-1$$

Images by MIT OpenCourseWare.

Quantum Mechanical Potentials

Particle in Free space



Gravitational lensing in the Abel 370 galaxy cluster. (Photo courtesy of NASA, ESA, the Hubble SM4 ERO Team and ST-ECF http://www.spacetelescope.org/images/heic0910b/.)

Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$$

Energy eigenvalues:

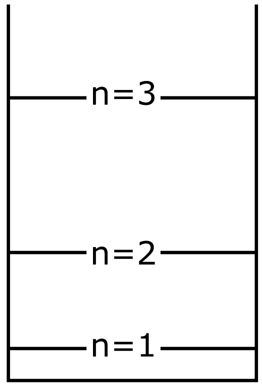
$$E_n = \frac{\hbar^2 k^2}{2m}$$

Energy eigenfunctions:

$$u_k(x) = e^{\pm ikx}$$

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

Particle in 1D box



Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$$V(x) = \begin{cases} 0, & 0 \le x \le d \\ \infty, & x > d \ \& \ x < 0 \end{cases}$$

Energy eigenvalues:

$$E_n = \frac{\hbar^2 \pi^2 n^2}{2md^2}$$

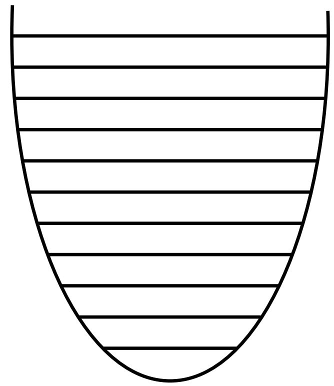
$$\Delta E_n = E_{n+1} - E_n = \frac{\hbar^2 \pi^2}{2md^2}(2n+1)$$

Energy eigenfunctions:

$$u_n(x) = A_n \sin\frac{n\pi x}{d}$$

$$A_n = \sqrt{\frac{2}{d}}$$

1D SHO



Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2} \quad m\omega^2 x^2$$

Energy eigenvalues:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

$$\Delta E_n = E_{n+1} - E_n = \hbar\omega$$

Energy eigenfunctions:

$$u_n(x) = e^{-\frac{m\omega}{2\hbar}x^2} h_n(x)$$

$$h_n(x) - Hermite\ polynomial$$

Periodic Potential

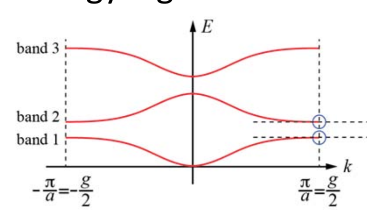
Figure removed due to copyright restrictions. See Fig. 3:Kittel, Charles. *Introduction to Solid State Physics*. 8th ed. Wiley 2004, p. 178.

Hamiltonian:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \sum_G V_G e^{iGx}$$

$$G = ng, \quad g = \frac{2\pi}{a}$$

Energy eigenvalues:



Energy eigenfunctions:

$$u_{n,k}(x) = e^{ikx}\sum_G C_{k-G} e^{-iGx}$$

$$-\frac{g}{2} \le x \le \frac{g}{2} \Rightarrow BZ$$

Images by MIT OpenCourseWare.

Carriers in Intrinsic Semiconductors

D.O.S.:

$$g_c(E) = \frac{m_c^{3/2}}{\pi^2\hbar^3}\sqrt{2(E-E_c)}$$

$$g_v(E) = \frac{m_v^{3/2}}{\pi^2\hbar^3}\sqrt{2(E_v-E)}$$

Carrier concentrations:

$$n = \int_{E_c}^{\infty} g_c(E) f(E)\, dE = N_C \exp\left(-\frac{E_C - E_F}{k_B T}\right)$$

$$p = \int_{-\infty}^{E_v} g_v(E)\left(1 - f(E)\right) dE = N_V \exp\left(-\frac{E_F - E_V}{k_B T}\right)$$

Fermi distribution function:

$$f_e(E) = \frac{1}{1 + e^{(E-E_F)/k_B T}}$$

$$f_h(E) = 1 - f_e(E) = \frac{1}{1 + e^{(E_F-E)/k_B T}}$$

Law of Mass Action:

$$np = N_C N_V \exp\left(-\frac{E_g}{k_B T}\right) = n_i^2, \quad n_i = \sqrt{N_C N_V}\exp\left(-\frac{E_g}{2k_B T}\right)$$

Intrinsic carrier concentration:

$$n_i(Si) = 10^{10}\, cm^{-3}$$

$$n_i(GaAs) = 2 \cdot 10^{6}\, cm^{-3}$$

Fermi level in Intrinsic SC:

$$n = p = n_i \Rightarrow \mu \equiv E_F = E_v + \frac{1}{2}E_g + \frac{3}{4}k_B T \ln\left(\frac{m_v^*}{m_c^*}\right)$$

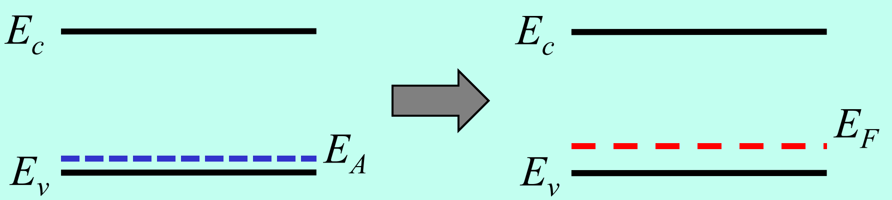
Extrinsic (Doped) Semiconductors

p-type

Figure removed due to copyright restrictions. Fig. 2.16: Pierret, Robert F. *Semiconductor Fundamentals*. 2nd ed. Prentice Hall, 1988.

$$p \sim N_A, \quad n \sim \frac{n_i^2}{N_A}$$

$$E_F = E_{Fi} - k_B T \ln\left(\frac{N_A}{n_i}\right)$$

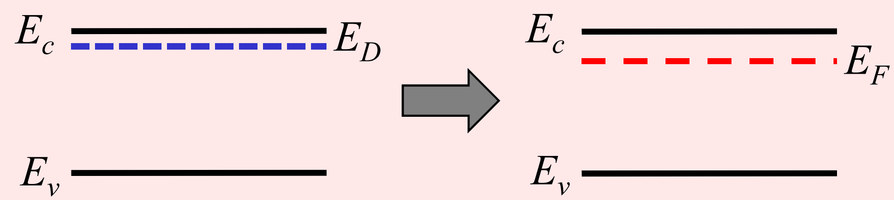


n-type

Figure removed due to copyright restrictions. Fig. 2.16: Pierret, Robert F. *Semiconductor Fundamentals*. 2nd ed. Prentice Hall, 1988.

$$n \sim N_D, \quad p \sim \frac{n_i^2}{N_D}$$

$$E_F = E_{Fi} + k_B T \ln\left(\frac{N_D}{n_i}\right)$$



Conductivity of SC: $\sigma = e n_c \mu_n + e p_v \mu_p$

Temperature dependence for *n*-type:

Figure removed due to copyright restrictions. Fig. 2.22: Pierret, Robert F. *Semiconductor Fundamentals*. 2nd ed. Prentice Hall, 1988.

PN Junction

W – depletion width

V_{bi} – built-in voltage

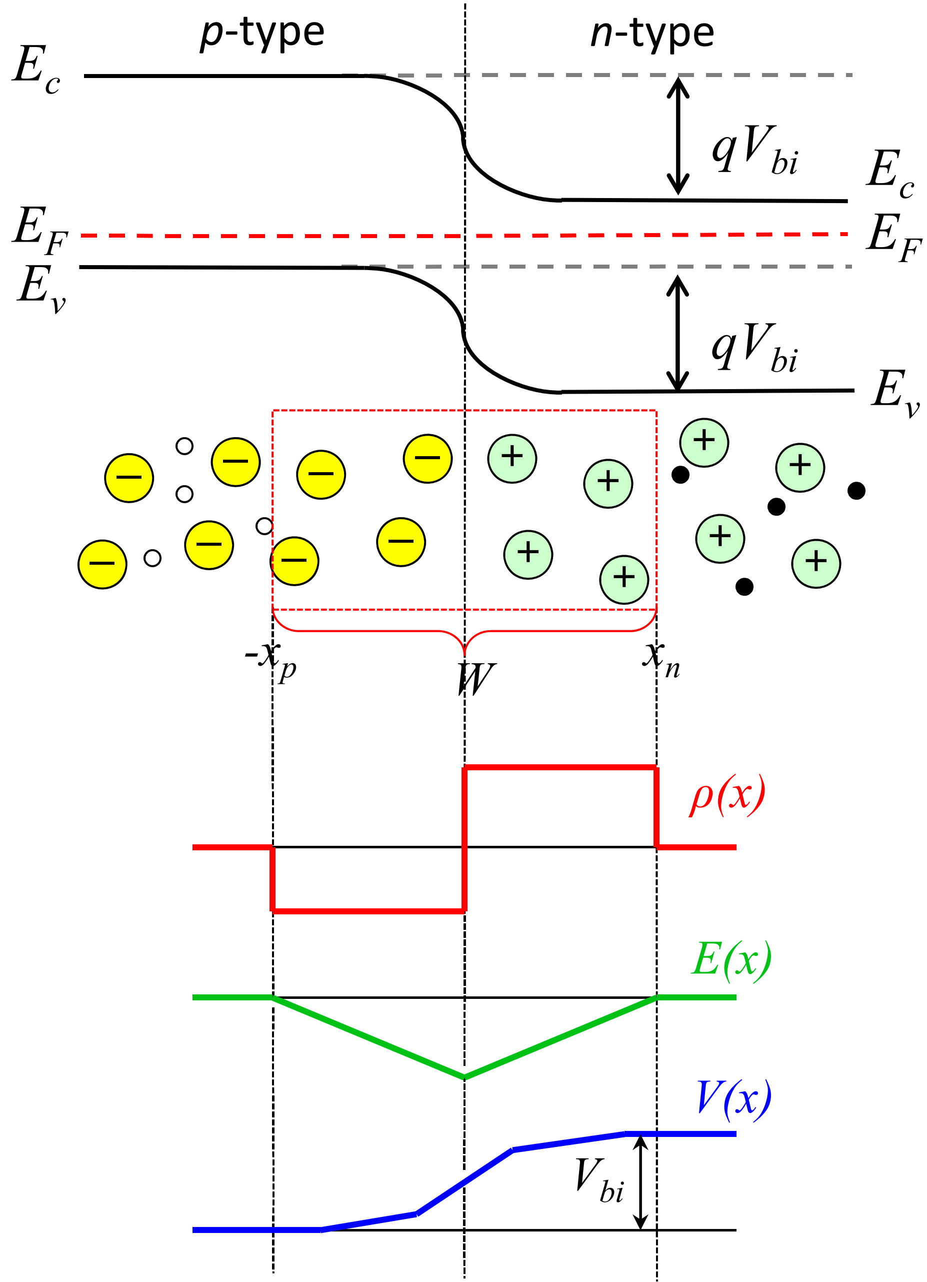
$$V_{bi} = E_F^n - E_F^p = \frac{k_B T}{e} \ln\left(\frac{N_D N_A}{n_i^2}\right)$$

$$N_D x_n = N_A x_p$$

$$x_p = \sqrt{\frac{2\varepsilon_r \varepsilon_0 V_{bi}}{e} \frac{N_D}{N_A (N_D + N_A)}}$$

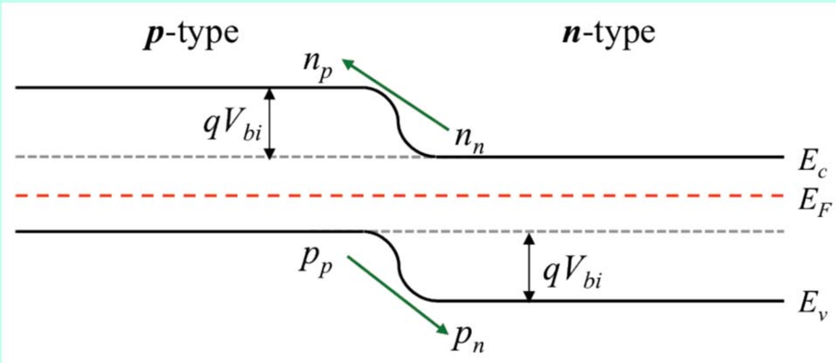
$$x_p = \sqrt{\frac{2\varepsilon_r \varepsilon_0 V_{bi}}{e} \frac{N_A}{N_D (N_D + N_A)}}$$

$$W = x_p + x_n = \sqrt{\frac{2\varepsilon_r \varepsilon_0 V_{bi}}{e} \frac{(N_D + N_A)}{N_D N_A}}$$



PN Junction Diodes: PVs and LEDs

Diode IV-characteristic



$$J = J_{diff} + J_{drift}$$

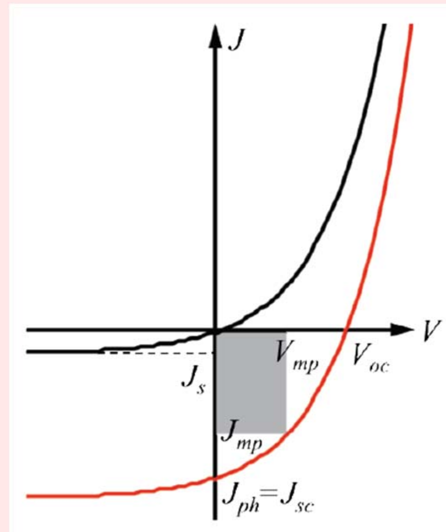
Forward bias: diffusion current

Reverse bias: drift current (J_s)

$$J = q\left(\frac{D_n}{L_n}\frac{n_i^2}{N_A} + \frac{D_p}{L_p}\frac{n_i^2}{N_D}\right)\left(e^{\frac{qV_a}{k_BT}} - 1\right) = J_s\left(e^{\frac{qV_a}{k_BT}} - 1\right)$$

Figure removed due to copyright restrictions. Fig. 15.1-18(c): Saleh, Bahaa E. A., and Malvin Carl Teich. *Fundamentals of Photonics*. 2nd ed. Wiley, 2007.

Photovoltaic cells:



$$J_{light} = J_s\left(e^{\frac{qV_a}{k_BT}} - 1\right) - J_{ph}$$

$$V_{oc} = \frac{k_BT}{q}\ln\left(\frac{J_{ph}}{J_s} + 1\right)$$

$$FF = \frac{V_{mp}J_{mp}}{V_{oc}J_{sc}}$$

Light Emitting Devices:

$$k_{sp}(\omega) = D\sqrt{\hbar\omega - E_g}\,e^{-(\hbar\omega - E_g)/k_BT}, \;\; where\; D = \frac{(2m_r)^{\frac{3}{2}}}{2\pi^2\hbar^2\tau_R}e^{(E_{Fc}-E_{Fv}-E_g)/k_BT}$$

Figure removed due to copyright restrictions. Fig. 16.1-4: Saleh, Bahaa E. A., and Malvin Carl Teich. *Fundamentals of Photonics*. 2nd ed. Wiley, 2007.

$$\hbar\omega_{peak} = E_g + \frac{1}{2}k_BT$$

Electromagnetic Waves in Materials

Maxwell's Equations:

$$\nabla\times\vec{E}=-\frac{\partial B}{\partial t}$$

$$\nabla\cdot\vec{D}=\rho_f$$

$$\nabla\times\vec{H}=\vec{J}_f+\frac{\partial\vec{D}}{\partial t}$$

$$\nabla\cdot\vec{B}=0$$

Constitutive Relations in Linear Media:

$$\vec{D}=\varepsilon_0\vec{E}+\vec{P}=\varepsilon_0(1+\chi)\vec{E}=\varepsilon_r\varepsilon_0\vec{E}=\varepsilon\cdot\vec{E}$$

$$\vec{B}=\varepsilon_0\vec{H}+\vec{M}=\varepsilon_0(1+\chi_m)\vec{H}=\mu_r\mu_0\vec{H}=\mu\cdot\vec{H}$$

Wave Equations:

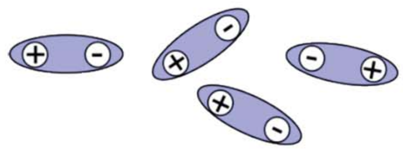
$$\left(\nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\vec{E}=0$$

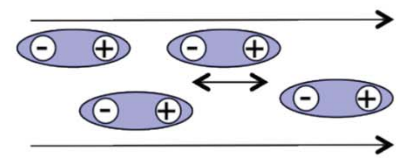
$$\left(\nabla^2-\frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right)\vec{B}=0$$

$$\vec{E}(\vec{r},t)=\vec{E}_0e^{i\vec{k}\vec{r}-i\omega t}+c.c.$$

$$\vec{H}(\vec{r},t)=\vec{H}_0e^{i\vec{k}\vec{r}-i\omega t}+c.c.$$

Damped oscillator model for polarization:





$$\frac{d^2\vec{P}}{dt^2}+\sigma\frac{d\vec{P}}{dt}+\omega_0^2\vec{P}=\omega_0^2\varepsilon_0\chi_0\vec{E}$$

$$\vec{P}=\frac{\omega_0^2\varepsilon_0\chi_0}{\omega_0^2-\omega^2-i\sigma\omega}\vec{E}=\varepsilon_0\chi(\omega)\vec{E}$$

$$\chi(\omega)=\chi'(\omega)+i\chi''(\omega)$$

$$\chi'(\omega)=\chi_0\frac{\omega_0^2\left(\omega_0^2-\omega^2\right)}{\left(\omega_0^2-\omega^2\right)^2+(\sigma\omega)^2}$$

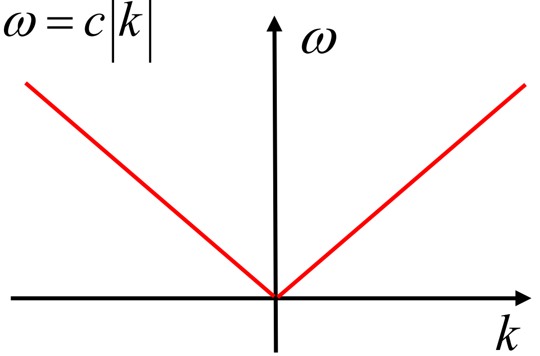
$$\chi''(\omega)=\chi_0\frac{\omega_0^2\sigma\omega}{\left(\omega_0^2-\omega^2\right)^2+(\sigma\omega)^2}$$

$$c=\frac{c_0}{n}=\frac{1}{\sqrt{\mu\varepsilon}},\quad c_0=\frac{1}{\sqrt{\mu_0\varepsilon_0}}\approx 3\times10^8\,\frac{m}{s}$$

Optical Interfaces: Continuity of Phase

Dispersion relation for photons:

$$\omega = c\left|\vec{k}\right|$$



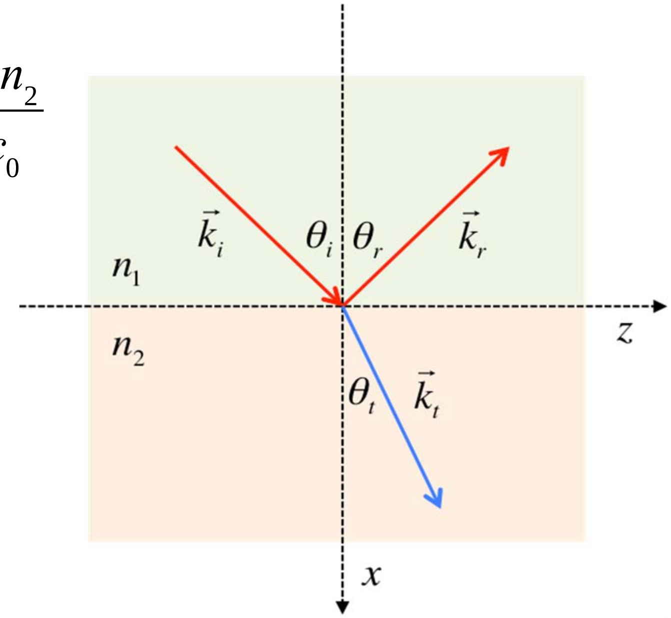
$$\left|\vec{k}_i\right| = \left|\vec{k}_r\right| = \frac{\omega n_1}{c_0}, \quad \left|\vec{k}_t\right| = \frac{\omega n_2}{c_0}$$

$$k_{iz} = k_{rz} = k_{tz} \equiv \beta$$

$$\theta_i = \theta_r$$

Snell's law:

$$n_1 \sin\theta_i = n_2 \sin\theta_t$$



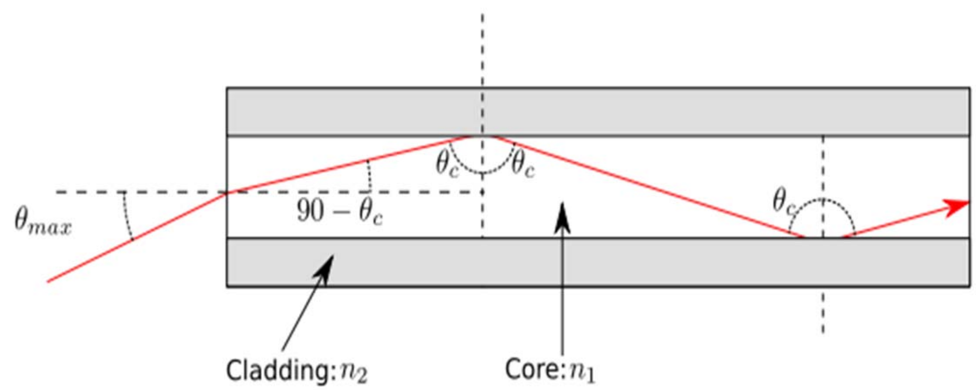
Total Internal Reflection:

$$\sin\theta_c = \frac{n_2}{n_1}\sin\theta_t = \frac{n_2}{n_1}$$

Numerical Aperture for a Waveguide:

$$NA = n \cdot \sin\theta_{\max} = \sqrt{n_1^2 - n_2^2}$$

For air: $n = 1$



Optical Interfaces: Boundary Conditions

Boundary Conditions:

$$\vec{E}_{1\parallel} = \vec{E}_{2\parallel}$$
$$D_{2\perp} - D_{1\perp} = \sigma$$
$$\vec{H}_{2\parallel} - \vec{H}_{1\parallel} = \vec{K}$$
$$B_{1\perp} = B_{2\perp}$$

$\sigma = 0$, $\vec{K} = 0$ ⇒

$$\vec{E}_{1\parallel} = \vec{E}_{2\parallel}$$
$$\varepsilon_2 E_{2\perp} = \varepsilon_1 E_{1\perp}$$
$$\vec{H}_{2\parallel} = \vec{H}_{1\parallel}$$
$$\mu_1 H_{1\perp} = \mu_2 H_{2\perp}$$

Reflection Coefficients:

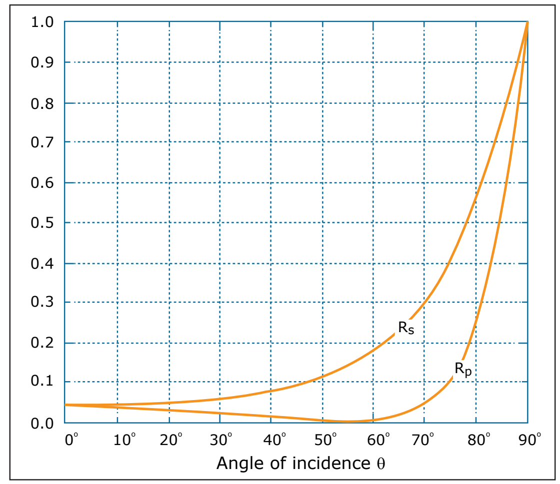
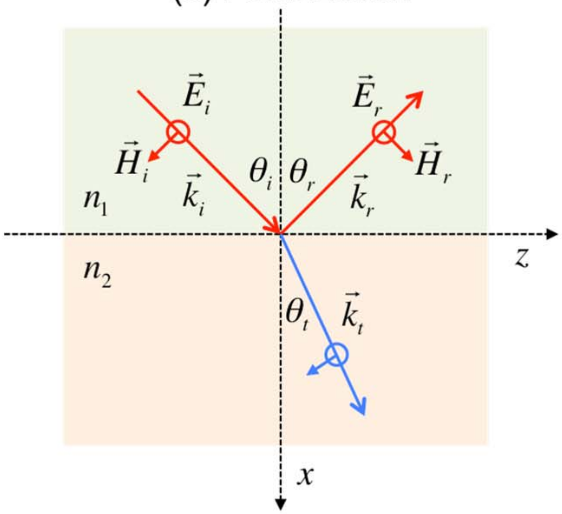


Image by MIT OpenCourseWare.

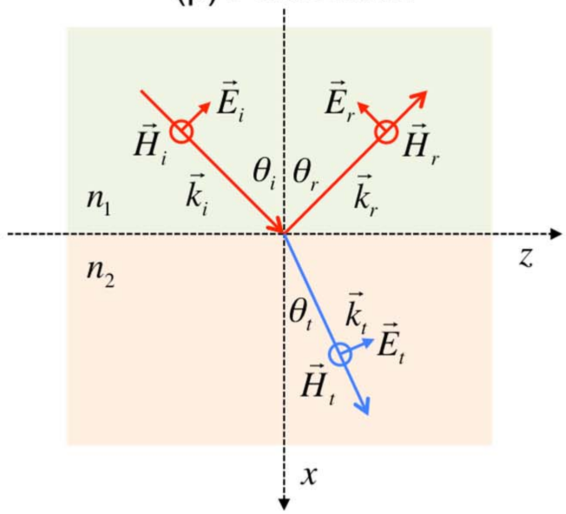
Brewster angle:

$$\sin^2\theta_B = \frac{n_2^2}{n_1^2 + n_2^2}$$

(s) Polarization



(p) Polarization



Antireflective coatings:

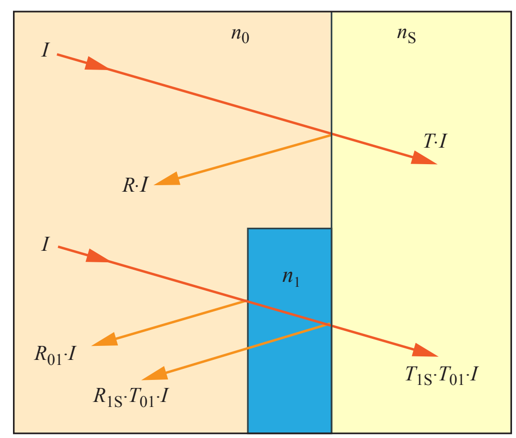
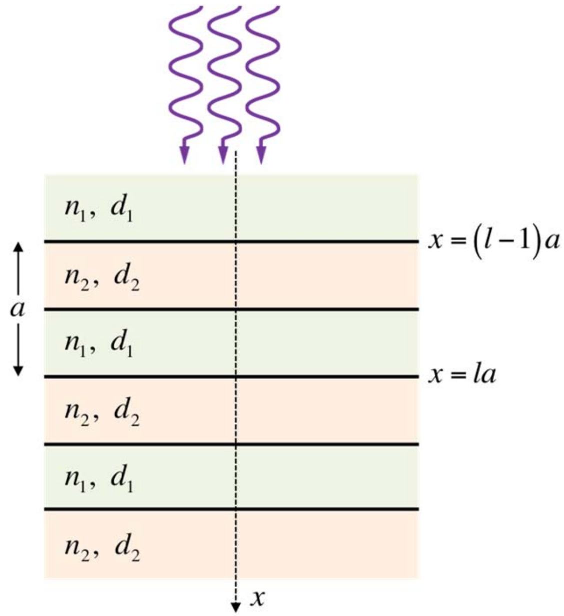


Image by MIT OpenCourseWare.

$$n_I = \sqrt{n_0 n_S} \qquad d = \frac{\lambda_0}{4n_I}$$

Periodic Optical Materials: Photonic Crystals



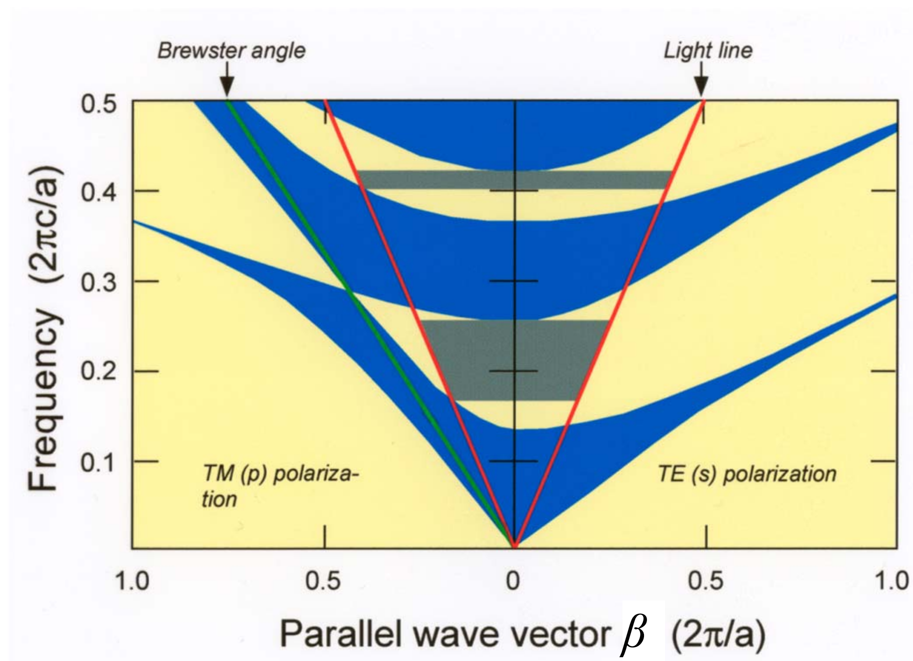
$$\begin{pmatrix} E_{1(l-1)} \\ E'_{1(l-1)} \end{pmatrix} = \underbrace{D_{21}P_2D_{12}P_1}_{M} \begin{pmatrix} E_{1l} \\ E'_{1l} \end{pmatrix}$$

$$\begin{pmatrix} E_{1(l-1)} \\ E'_{1(l-1)} \end{pmatrix} = e^{-iKa} \begin{pmatrix} E_{1l} \\ E'_{1l} \end{pmatrix}$$

$$M \begin{pmatrix} E_{1l} \\ E'_{1l} \end{pmatrix} = e^{-iKa} \begin{pmatrix} E_{1l} \\ E'_{1l} \end{pmatrix}$$

$$k_z = \beta = 0$$

Figure removed due to copyright restrictions. Bloch waves corresponding to the A and B solutions for frequency at the edge of the Brillouin zone: Unknown source.

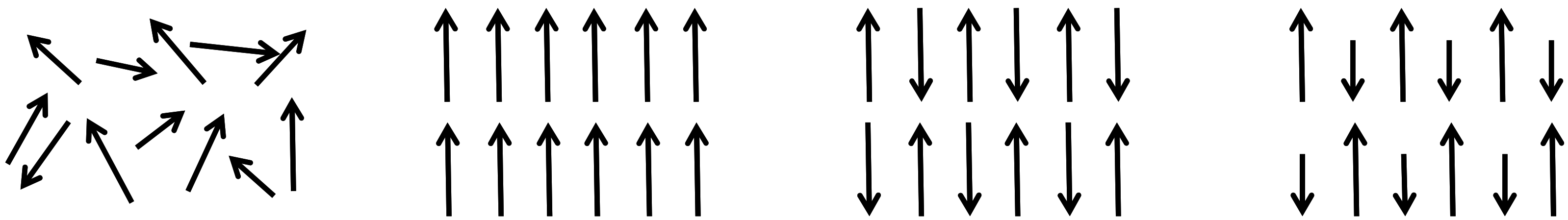


$$g = \frac{2\pi}{a},\ \ a = d_1 + d_2$$

Classification of Magnetic Materials

Exchange interaction: $E_{ex} = -2J_{ex}\vec{S}_1\vec{S}_2$

Paramagnetic | Ferromagnetic | Anti-Ferromagnetic | Ferrimagnetic



$J_{ex} = 0$ | $J_{ex} > 0$ | $J_{ex} < 0$ | $J_{ex} < 0$

Magneto crystalline anisotropy energy:

$$E_a = \sum_n K_{un} \sin^{2n}\theta \approx K_u \sin^2\theta$$

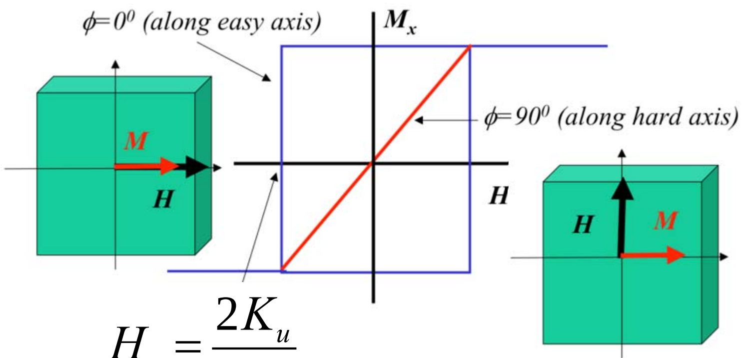
Easy axis: low magnetic field needed to magnetize to saturation

Hard axis: high magnetic field needed to magnetize to saturation

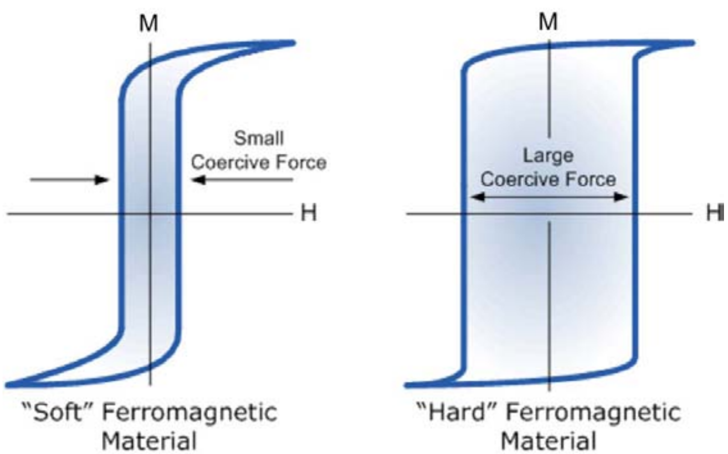
Mn, Fe, Ni – cubic, low anisotropy
Co – hexagonal, high anisotropy

Hysteresis in Ferromagnetic Materials

Single domain ferromagnet:



$$H_c = \frac{2K_u}{M_s}$$



Courtesy of Wayne Storr. Used with permission.

Soft: low anisotropy, easy to magnetize (transformers, generators)

Hard: high anisotropy, hard to magnetize (hard drives, permanent magnets)

Domains and domain walls

Domain wall width: $\delta = Na = \pi S\sqrt{\frac{2J}{K_u a^3}} \Rightarrow \begin{cases} J\uparrow \Rightarrow \delta\uparrow \\ K_u\uparrow \Rightarrow \delta\downarrow \end{cases}$

Domain wall energy: $\sigma_{BW} = \pi S\sqrt{\frac{2JK_u}{a}}$

Types of walls:

Figure removed due to copyright restrictions. Bloch wall and Neél wall: O'Handley, Robert C. *Modern Magnetic Materials*. Wiley, 1999.

Domain wall motion: