

ECE 109: Principles of Electronic Materials

Study Reference — Key Equations with Variable Definitions (Lessons 1–6)

Physical Constants

h	$6.626 \times 10^{-34} \text{ J s}$
$\hbar = h/2\pi$	$1.055 \times 10^{-34} \text{ J s}$
hc	1240 eV nm
m_e	$9.109 \times 10^{-31} \text{ kg}$
e	$1.602 \times 10^{-19} \text{ C}$
k_B	$1.381 \times 10^{-23} \text{ J/K}$ $= 8.617 \times 10^{-5} \text{ eV/K}$
ϵ_0	$8.854 \times 10^{-12} \text{ F/m}$
μ_0	$4\pi \times 10^{-7} \text{ N/A}^2$
c_0	$3.0 \times 10^8 \text{ m/s}$
N_A	$6.022 \times 10^{23} \text{ mol}^{-1}$
a_0	$0.0529 \text{ nm (Bohr radius)}$
$\frac{e^2}{4\pi\epsilon_0}$	1.44 eV nm
$k_B T _{300\text{K}}$	0.02585 eV

Wave–Particle Duality

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

f = frequency, $\omega = 2\pi f$ = angular frequency

$$p = \frac{h}{\lambda} = \frac{\hbar f}{c}$$

p = photon momentum, λ = wavelength

$$\text{Photoelectric: } KE_{\max} = hf - \Phi$$

Φ = work function (min. energy to free electron)

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2m_e eV}}$$

de Broglie λ for electron accelerated through V

Schrödinger Equation

$$\text{Momentum op. } \hat{p} = -i\hbar \frac{\partial}{\partial x}$$

$$\text{Expectation } \langle A \rangle = \int \psi^* \hat{A} \psi dx$$

$\hat{A}$ = quantum operator for observable A

$$\text{Normalization } \int_{-\infty}^{\infty} |\psi|^2 dx = 1$$

$$\text{TDSE } i\hbar \frac{\partial}{\partial t} |\psi\rangle = \hat{H} |\psi\rangle$$

$$\text{Hamiltonian } \hat{H} = -\frac{\hbar^2}{2m} \nabla^2 + V(\mathbf{r})$$

$\hat{H}$ = Hamiltonian (total energy operator)

$$\text{TISE } \frac{d^2\psi}{dx^2} + \frac{2m_e}{\hbar^2} (E - V) \psi = 0$$

V = potential energy, E = total energy

Infinite Potential Well

$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$E_n = \frac{n^2 \pi^2 \hbar^2}{2m_e a^2} = \frac{n^2 \hbar^2}{8m_e a^2}$$

a = well width, $n = 1, 2, 3, \dots$

$$|\psi_n|^2 = \frac{2}{a} \sin^2\left(\frac{n\pi x}{a}\right)$$

$$\Delta E_n = E_{n+1} - E_n = \frac{(2n+1)\hbar^2}{8m_e a^2}$$

$$\text{3D box } E_{n_1 n_2 n_3} = \frac{\hbar^2}{8m_e} \left(\frac{n_1^2}{a^2} + \frac{n_2^2}{b^2} + \frac{n_3^2}{c^2} \right)$$

a, b, c = box dimensions along x, y, z

Finite Potential Well

$$k^2 = \frac{2m_e E}{\hbar^2}, \quad \alpha^2 = \frac{2m_e (V_0 - E)}{\hbar^2}$$

k = wavevector inside well, α = decay const. outside

$$\text{Even } \alpha = k \tan\left(\frac{ka}{2}\right)$$

$$\text{Odd } \alpha = -k \cot\left(\frac{ka}{2}\right)$$

Transcendental eqs solved graphically for bound states

$$\text{Penetration } \delta = \frac{1}{\alpha} = \frac{\hbar}{\sqrt{2m_e (V_0 - E)}}$$

δ = penetration depth into classically forbidden region

$$\text{Bound states } N \leq \left\lfloor \frac{1}{2} + \frac{a}{\pi} \sqrt{\frac{2m_e V_0}{\hbar^2}} \right\rfloor$$

Quantum Tunneling

$$T = \frac{1}{1 + D \sinh^2(\alpha a)}$$

$$D = \frac{V_0^2}{4E(V_0 - E)}, \quad \alpha = \frac{\sqrt{2m_e(V_0 - E)}}{\hbar}$$

T = transmission prob., V_0 = barrier height, a = barrier width

$$\text{Thick barrier } T \approx T_0 e^{-2\alpha a}, \quad T_0 = \frac{16E(V_0 - E)}{V_0^2}$$

Valid when $\alpha a \gg 1$ (opaque barrier)

$$\text{STM current } I \propto V_b e^{-2\alpha d}, \quad \alpha = \frac{\sqrt{2m_e \phi}}{\hbar}$$

V_b = bias, d = tip–sample gap, ϕ = avg. work function

Uncertainty Principle

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}, \quad \Delta E \cdot \Delta t \geq \frac{\hbar}{2}$$

$\Delta x, \Delta p$ = std. dev. of position/momentum

Hydrogen Atom

$$V(r) = \frac{-Ze^2}{4\pi\epsilon_0 r}$$

Z = atomic number (1 for hydrogen)

$$E_n = \frac{-13.6 \text{ eV}}{n^2}$$

n = principal quantum number

$$L = \hbar \sqrt{\ell(\ell+1)}, \quad L_z = m_\ell \hbar$$

ℓ = orbital angular momentum quantum number

$$S = \hbar \sqrt{s(s+1)} = \frac{\sqrt{3}}{2} \hbar, \quad S_z = m_s \hbar$$

Quantum numbers: $n = 1, 2, \dots$; $\ell = 0 \dots n-1$; $m_\ell = -\ell \dots +\ell$; $m_s = \pm \frac{1}{2}$

Degeneracy: n^2 orbitals, $2n^2$ states per shell

$$\text{Selection rules } \Delta \ell = \pm 1, \Delta m_\ell = 0, \pm 1$$

Governs allowed electric dipole transitions

$$\text{Virial } \langle T \rangle = -E, \quad \langle V \rangle = 2E$$

Relates average kinetic/potential energy to total energy

Interatomic Bonding

$$E(r) = -\frac{A}{r} + \frac{B}{r^m}$$

A = attractive const., B = repulsive const., $m \approx 6-12$

Ionic $A = \frac{Me^2}{4\pi\epsilon_0}$

M = Madelung constant (geometry-dependent)

$$E_{\text{lattice}}(r) = -\frac{Me^2}{4\pi\epsilon_0 r} + \frac{B}{r^m}$$
$$E_{\text{bond}} = \frac{A}{r_0} \left(1 - \frac{1}{m}\right)$$

r_0 = equilibrium bond distance where $dE/dr = 0$

$$r_0 = \left(\frac{mB \cdot 4\pi\epsilon_0}{e^2 M}\right)^{1/(m-1)}$$

Crystal Structures

	atoms	CN	APF	$r(a)$
SC	1	6	0.52	$a/2$
BCC	2	8	0.68	$a\sqrt{3}/4$
FCC	4	12	0.74	$a\sqrt{2}/4$
DC	8	4	0.34	$a\sqrt{3}/8$

CN = coordination number, APF = atomic packing fraction, r = atomic radius, a = lattice constant

Density $\rho = \frac{n_c M_a}{N_A a^3}$

n_c = atoms per unit cell, M_a = molar mass

NaCl $M = 1.748$ **CsCl** $M = 1.763$

Surface $\sigma_{100} = \frac{2}{a^2}$, $\sigma_{110} = \frac{2\sqrt{2}}{a^2}$, $\sigma_{111} = \frac{4}{\sqrt{3}a^2}$

σ_{hkl} = planar atomic density for FCC [atoms/area]

X-ray Diffraction

$$d_{hkl} = \frac{a}{\sqrt{h^2 + k^2 + l^2}}$$

d_{hkl} = spacing between (hkl) planes

$$2d \sin \theta = n\lambda \quad (\text{Bragg's law})$$

θ = diffraction angle, n = order, λ = X-ray wavelength

Systematic absences:

BCC: $h+k+l$ = even

FCC: h, k, l all odd or all even

Crystal Defects

$$n_v = N \exp\left(-\frac{E_v}{k_B T}\right)$$

n_v = vacancy conc., N = atomic sites per volume, E_v = formation energy

Stoichiometry

$$w_A = \frac{x M_A}{x M_A + y M_B}, \quad x_i = \frac{n_i}{\sum_j n_j}$$

w_A = weight fraction, x_i = mole fraction

Band Theory

$$E_g = E_c - E_v$$

E_g = band gap, E_c = conduction band edge, E_v = valence band edge

Photoemission

Metal: $hf > \Phi$, $KE = hf - \Phi$

Semiconductor: $hf > E_g + \chi$

χ = electron affinity (vacuum level to E_c)

E-k Dispersion & Effective Mass

$$E = \frac{\hbar^2 k^2}{2m_e^*}$$

Parabolic approx. near band extrema; k = crystal wavevector

$$\frac{1}{m_e^*} = \frac{1}{\hbar^2} \frac{d^2 E}{dk^2}$$

m_e^* = effective mass (from band curvature)

$$\left(\frac{1}{m^*}\right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E}{\partial k_i \partial k_j}$$

Density of States

$$g(E) = 8\pi\sqrt{2} \left(\frac{m_e}{\hbar^2}\right)^{3/2} E^{1/2}$$

$g(E)$ = states per unit energy per unit volume

$$S_v(E') = \frac{\pi(8m_e E')^{3/2}}{3h^3}$$

S_v = cumulative states up to energy E'

Fermi-Dirac Statistics

$$f(E) = \frac{1}{1 + \exp\left(\frac{E - E_F}{k_B T}\right)}$$

$f(E)$ = occupation probability; E_F = Fermi energy

Boltzmann approx. $f \approx e^{-(E-E_F)/(k_B T)}$ for $E - E_F \gg k_B T$

Boltzmann ratio $\frac{N_2}{N_1} = \exp\left(-\frac{E_2 - E_1}{k_B T}\right)$

$$E_{F0} = \frac{\hbar^2}{8m_e} \left(\frac{3n}{\pi}\right)^{2/3}$$

E_{F0} = Fermi energy at $T = 0$; n = electron concentration

$$E_F(T) = E_{F0} \left[1 - \frac{\pi^2}{12} \left(\frac{k_B T}{E_{F0}}\right)^2\right]$$

$$\bar{E} = \frac{3}{5} E_{F0}$$

Average electron energy at $T = 0$

Fermi vel. $v_F = \sqrt{2E_F/m_e}$

Thermal vel. $v_{\text{rms}} = \sqrt{3k_B T/m_e}$

Drude Model & Conduction

$$v_F = \sqrt{\frac{2E_F}{m_e}}, \quad l = v_F \tau$$

v_F = Fermi velocity, l = mean free path, τ = mean free time

$$v_{dx} = \frac{eE_x}{m_e} \tau = \mu E_x$$

v_{dx} = drift velocity in applied field E_x

$$\mu = \frac{e\tau}{m_e}$$

μ = electron mobility [$\text{m}^2/(\text{V s})$]

$$J_x = en v_{dx} = \sigma E_x$$

J_x = current density, n = electron concentration

$$\sigma = \frac{ne^2\tau}{m_e} = ne\mu$$

σ = conductivity [S/m]

$$R = \frac{\rho L}{A}, \quad \rho = \frac{1}{\sigma}$$

R = resistance, ρ = resistivity, L = length, A = area

Band model $\sigma = \frac{1}{3}e^2 v_F^2 \tau g(E_F)$

Electron conc. $n = \frac{Z \cdot d \cdot N_A}{M_{at}}$

Z = valence, d = mass density, M_{at} = atomic mass

Mean free time $\tau = \frac{m_e}{ne^2\rho}$

Thermoelectrics

$$S = \frac{dV}{dT} \quad (\text{Seebeck coeff.})$$

S = Seebeck coefficient [V/K]

$$V_{AB} = \int_{T_0}^T (S_A - S_B) dT$$

V_{AB} = thermocouple voltage between materials A, B

Contact potential $\Delta V = \frac{\Phi_1 - \Phi_2}{e}$

Voltage from work function difference at junction

Maxwell's Equations

$$\nabla \cdot \vec{D} = \rho_{\text{free}}$$

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

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

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

EM Waves & Optics

$$\nabla^2 \mathbf{E} - \frac{1}{c^2} \frac{\partial^2 \mathbf{E}}{\partial t^2} = 0$$

$$c_0 = \frac{1}{\sqrt{\epsilon_0 \mu_0}}, \quad n = \sqrt{\epsilon_r}, \quad c = \frac{c_0}{n}$$

n = refractive index, ϵ_r = relative permittivity

$$\vec{D} = \epsilon_0 \vec{E} + \vec{P} = \epsilon_r \epsilon_0 \vec{E}$$

$\vec{P}$ = polarization, $\vec{D}$ = displacement field

Sellmeier $n^2(\lambda) = 1 + \sum_i \frac{B_i \lambda^2}{\lambda^2 - C_i}$

B_i, C_i = material-specific Sellmeier coefficients

$$v_g = \frac{c}{N_g}, \quad N_g = n - \lambda \frac{dn}{d\lambda}$$

v_g = group velocity, N_g = group index

Snell's Law & Fresnel

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

θ_i = incidence, θ_t = transmission angle

$$R_s = \left(\frac{n_1 \cos \theta_i - n_2 \cos \theta_t}{n_1 \cos \theta_i + n_2 \cos \theta_t} \right)^2$$

R_s = reflectance, s-polarized ($\perp$ plane of incidence)

$$R_p = \left(\frac{n_2 \cos \theta_i - n_1 \cos \theta_t}{n_2 \cos \theta_i + n_1 \cos \theta_t} \right)^2$$

R_p = reflectance, p-polarized ($\parallel$ plane of incidence)

Normal inc. $R = \left(\frac{n_1 - n_2}{n_1 + n_2} \right)^2$

$$\tan \theta_B = \frac{n_2}{n_1} \quad (\text{Brewster})$$

θ_B = Brewster angle ($R_p = 0$)

$$\theta_c = \arcsin\left(\frac{n_2}{n_1}\right) \quad (\text{Critical})$$

θ_c = critical angle for TIR ($n_1 > n_2$)

Absorption & Attenuation

$$I(z) = I_0 e^{-\alpha z}$$

α = absorption coefficient [Np/m]

$$\alpha = \frac{\pi \epsilon_r''}{\lambda \sqrt{\epsilon_r'}}$$

$$\frac{P_{\text{out}}}{P_{\text{in}}} = e^{-2\alpha z}$$

Power (not field) attenuation uses 2α

Wave Properties

Plane wave $E(z, t) = E_0 \cos(kz - \omega t + \phi_0)$

$$k = \frac{2\pi}{\lambda}, \quad \omega = 2\pi f, \quad v = f\lambda = \frac{\omega}{k}$$

k = wavenumber, ω = angular frequency

Standing wave $E = 2E_0 \cos(kz) \cos(\omega t)$

Antinode spacing = $\lambda/2$

Electric Polarization

$$\mathbf{D} = \epsilon_0 \mathbf{E} + \mathbf{P} = \epsilon_r \epsilon_0 \mathbf{E}$$
$$\mathbf{P} = \chi_e \epsilon_0 \mathbf{E}, \quad \epsilon_r = 1 + \chi_e$$

χ_e = electric susceptibility

$$\mathbf{P} = N \cdot \mathbf{p}_{\text{avg}}$$

N = number density, $\mathbf{p}_{\text{avg}}$ = avg. dipole moment per unit

$$\mathbf{p} = \alpha_e \mathbf{E}_{\text{loc}}$$

α_e = polarizability, $\mathbf{E}_{\text{loc}}$ = local field

$$\mathbf{E}_{\text{loc}} = \mathbf{E} + \frac{\mathbf{P}}{3\epsilon_0}$$

Lorentz local field (includes depolarization from surroundings)

Clausius–Mossotti

$$\frac{\epsilon_r - 1}{\epsilon_r + 2} = \frac{N\alpha_e}{3\epsilon_0}$$

Relates macroscopic ϵ_r to microscopic polarizability α_e

$$\text{Rearranged: } \alpha_{\text{total}} = \frac{3\epsilon_0(\epsilon_r - 1)}{N(\epsilon_r + 2)}$$

Polarizability Mechanisms

$$\alpha_{\text{total}} = \alpha_e + \alpha_i + \alpha_d$$

electronic + ionic + orientational (dipolar)

$$\alpha_e = 4\pi\epsilon_0 R^3 \quad (\text{electronic})$$

R = atomic/ionic radius

$$\alpha_d = \frac{p^2}{3k_B T} \quad (\text{orientational})$$

p = permanent dipole moment; dominates at low ω

$$\text{Langevin } L(x) = \coth(x) - \frac{1}{x}, \quad x = \frac{pE}{kT}$$

Exact orientational polarization; α_d is the weak-field limit

Optical Permittivity

At optical freq., only α_e contributes:

$$\alpha_{\text{opt}} = \alpha_e(\text{cation}) + \alpha_e(\text{anion})$$

$$\frac{\epsilon_{\text{rop}} - 1}{\epsilon_{\text{rop}} + 2} = \frac{N\alpha_{\text{opt}}}{3\epsilon_0}$$

ϵ_{rop} = optical (high-freq.) relative permittivity

Debye Relaxation

$$\epsilon_r(\omega) = \epsilon_{r\infty} + \frac{\epsilon_{rs} - \epsilon_{r\infty}}{1 + j\omega\tau}$$

ϵ_{rs} = static (DC), $\epsilon_{r\infty}$ = high-freq. permittivity, τ = relaxation time

$$\epsilon'_r = \epsilon_{r\infty} + \frac{\epsilon_{rs} - \epsilon_{r\infty}}{1 + \omega^2\tau^2}$$

$$\epsilon''_r = \frac{(\epsilon_{rs} - \epsilon_{r\infty})\omega\tau}{1 + \omega^2\tau^2}$$

ϵ'_r = storage (real), ϵ''_r = loss (imaginary)

$$\tan \delta = \frac{\epsilon''_r}{\epsilon'_r}$$

Loss tangent; energy dissipated / stored per cycle

$$\text{Complex } \epsilon \quad \epsilon_r(\omega) = \epsilon'_r(\omega) - j\epsilon''_r(\omega)$$

$$\text{Complex } k \quad \tilde{k} = \frac{\omega}{c} \sqrt{\epsilon_r} = k' + ik''$$

Wave in Lossy Medium

$$E(z) = E_0 e^{-k''z} e^{i(k'z - \omega t)}$$

k'' = imaginary part of wavevector (attenuation)

Gauss's Law for D

$$\nabla \cdot \mathbf{D} = \rho_{\text{free}}$$

$$\oint \mathbf{D} \cdot d\mathbf{A} = Q_{\text{free, enclosed}}$$

$$\text{Boundary } D_{n1} - D_{n2} = \sigma_f$$

σ_f = free surface charge density at interface

Capacitors & Energy

$$C = \frac{\epsilon_r \epsilon_0 A}{d}$$

C = capacitance, A = plate area, d = separation

$$U = \frac{1}{2} CV^2 = \frac{1}{2} \epsilon_r \epsilon_0 E^2 \cdot (\text{Vol})$$

$$u = \frac{1}{2} \epsilon_r \epsilon_0 E^2 = \frac{1}{2} \mathbf{D} \cdot \mathbf{E}$$

u = energy density [J/m³]

Piezoelectricity

$$P = d \cdot T \quad (\text{direct}), \quad S = d \cdot E \quad (\text{converse})$$

d = piezoelectric coeff., T = stress, S = strain

$$f = \frac{v}{2L} \quad (\text{resonance}), \quad Q = \frac{f_{\text{res}}}{\Delta f}$$

v = acoustic velocity, L = crystal thickness, Q = quality factor

Number Density (Ionic Crystals)

$$N = \frac{n_c}{a^3}$$

e.g. NaCl: n_c = 4 ion pairs per unit cell

Useful Identities

$$1 \text{ eV} = 1.602 \times 10^{-19} \text{ J}$$

$$1 \text{ nm} = 10^{-9} \text{ m} = 10 \text{ \AA}$$

$$E = hf = hc/\lambda; \text{ at } \lambda = 1240 \text{ nm}, E = 1 \text{ eV}$$

$$\text{Euler } e^{i\theta} = \cos \theta + i \sin \theta$$

$$\sinh(x) = (e^x - e^{-x})/2, \quad \cosh(x) = (e^x + e^{-x})/2$$