Solid State Formula Sheet: Foundations, Bands, Carriers

Math and Statistics

$$n_B(\varepsilon) = \frac{1}{e^{\beta\varepsilon} - 1}, \qquad f(E) = \frac{1}{e^{(E-\mu)/(k_B T)} + 1}.$$

State density in k-space: $(L/2\pi)^d$ per branch; include degeneracy separately. Shell measures: $2\,dk$, $2\pi k\,dk$, $4\pi k^2\,dk$ in 1D, 2D, 3D.

$$\sin(\alpha \pm \beta) = \sin\alpha\cos\beta \pm \cos\alpha\sin\beta$$

$$\cos(\alpha \pm \beta) = \cos\alpha\cos\beta \mp \sin\alpha\sin\beta$$

$$\sin 2\theta = 2\sin\theta\cos\theta, \quad \cos 2\theta = 1 - 2\sin^2\theta = 2\cos^2\theta - 1$$

$$1 - \cos x = 2\sin^2(x/2), \quad 1 + \cos x = 2\cos^2(x/2).$$

$$\cos A + \cos B = 2\cos\frac{A+B}{2}\cos\frac{A-B}{2}.$$

Taylor: $e^x \simeq 1 + x$, $\sin x \simeq x$, $\cos x \simeq 1 - x^2/2$, $(1+x)^\alpha \simeq 1 + \alpha x$.

Einstein and Debye

Einstein: independent oscillators at one ω_0; Debye: elastic continuum, acoustic $\omega = v_s k$ with cutoff for $3N$ modes.

$$T_E = \hbar\omega_0/k_B$$

$$C_E = k_B\left(\frac{T_E}{T}\right)^2 \frac{e^{T_E/T}}{(e^{T_E/T} - 1)^2}.$$

$$C_D = 9Nk_B\left(\frac{T}{T_D}\right)^3 \int_0^{T_D/T} \frac{x^4 e^x}{(e^x - 1)^2}\,dx$$

$$x = \frac{\hbar\omega}{k_B T}.$$

Limits: $C_p \approx 3Nk_B$ at high T; $C_p \propto T^3$ near 0.

Harmonic Approximation

$$U \simeq U_0 + \frac{1}{2}\kappa(r - r_0)^2, \qquad F = -\kappa(r - r_0)$$

$$F = -\kappa a\frac{\delta L}{L}, \qquad \beta = -\frac{1}{L}\frac{\partial L}{\partial F} = \frac{1}{\kappa a}$$

$$v_s = \sqrt{\frac{1}{\rho\beta}} = \sqrt{\frac{\kappa a^2}{m}}.$$

Drude Transport

Classical free carriers with relaxation time τ; ignores Pauli filling and bands.

$$m\dot{\mathbf{v}} = -m\mathbf{v}/\tau - e(\mathbf{E} + \mathbf{v}\times\mathbf{B})$$

$$\mathbf{j} = -en\mathbf{v} = \sigma\mathbf{E}, \quad \sigma = \frac{ne^2\tau}{m} = ne\mu, \quad \rho_{xx} = \frac{m}{ne^2\tau}$$

$$\rho_{xy} = -\rho_{yx} = \frac{B}{ne} = -R_H B, \qquad R_H = -\frac{1}{ne}.$$

Sommerfeld Electrons

Quantum free-electron gas; thermodynamics comes from a $k_B T$ shell near E_F.

$$\varepsilon(k) = \frac{\hbar^2 k^2}{2m}, \qquad p_F = \hbar k_F, \qquad v_F = \frac{\hbar k_F}{m}$$

$$k_F = (3\pi^2 N/V)^{1/3}, \qquad \varepsilon_F = \frac{\hbar^2 k_F^2}{2m}, \qquad T_F = \varepsilon_F/k_B.$$

$T = 0$: filled up to ε_F; for metals at room $T \ll T_F$, $\mu \simeq \varepsilon_F$.

$$g_{3D}(\varepsilon) = \frac{Vm^{3/2}\sqrt{2\varepsilon}}{\pi^2\hbar^3}, \qquad C_e \approx 3Nk_B\frac{T}{T_F} \propto T.$$

Electronic heat: $U_e = \int E\,g(E)f(E)\,dE$, $C_e = dU_e/dT$. Parabolic DOS: $g_{1D} \propto \varepsilon^{-1/2}$, $g_{2D} =$ const., $g_{3D} \propto \sqrt{\varepsilon}$.

Bands, DOS, Effective Mass

$$v_g = \frac{1}{\hbar}\frac{\partial E}{\partial k}, \qquad m^* = \hbar^2\left(\frac{\partial^2 E}{\partial k^2}\right)^{-1}$$

$$g(E) = \frac{dN}{dE} = \frac{dN}{dk}\left|\frac{dk}{dE}\right|, \qquad g_{1D} = \frac{L}{\pi}\left|\frac{dk}{dE}\right|$$

$$g_{2D} = \frac{Ak}{2\pi}\left|\frac{dk}{dE}\right|, \qquad g_{3D} = \frac{Vk^2}{2\pi^2}\left|\frac{dk}{dE}\right|$$

per branch, before spin/valley degeneracy. For phonons use $E = \hbar\omega$: $g(\omega) = \hbar g(E)$. Van Hove singularities occur where $v_g = 0$.

LCAO and Tight Binding

Localized orbitals; weak hopping broadens atomic levels into bands. For two identical orbitals,

$$H_{\text{eff}} = \begin{pmatrix} E_0 & -t \\ -t & E_0 \end{pmatrix}, \qquad |\psi_\pm\rangle = \frac{|1\rangle \pm |2\rangle}{\sqrt{2}}$$

$$E_\pm = E_0 \mp t.$$

For $t > 0$, ψ_+ bonding, ψ_- antibonding. A 1D chain:

$$E(k) = E_0 - 2t\cos(ka), \qquad E_0 - 2t < E < E_0 + 2t$$

$$E \simeq E_0 - 2t + t(ka)^2, \qquad m^* = \frac{\hbar^2}{2ta^2}.$$

One band from N atoms holds $2N$ electrons incl. spin. More atoms/cell give more branches; phonons split into acoustic/optical branches.

Bloch and Nearly Free Electrons

Weak periodic potential; gaps open where free-electron states differ by $\mathbf{G}$.

$$H = \begin{pmatrix} E_0 + v\hbar\delta k & W \\ W^* & E_0 - v\hbar\delta k \end{pmatrix}$$

$$E_\pm = E_0 \pm \sqrt{(v\hbar\delta k)^2 + |W|^2}, \qquad \Delta E = 2|W|$$

$$W = V_G = \frac{1}{a}\int_0^a e^{-iGx}V(x)\,dx.$$

Periodic potentials couple states differing by $\mathbf{G}$. Bloch:

$$\psi^\alpha_{\mathbf{k}}(\mathbf{r}) = u^\alpha_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{r}}, \quad u^\alpha_{\mathbf{k}}(\mathbf{r} + \mathbf{R}) = u^\alpha_{\mathbf{k}}(\mathbf{r}).$$

$E^\alpha(\mathbf{k})$ is periodic under $\mathbf{k} \to \mathbf{k} + \mathbf{G}$.

Solid State Formula Sheet: Crystals, Doping, Devices

Crystal Structure

$$\mathbf{R} = n_1\mathbf{a}_1 + n_2\mathbf{a}_2 + n_3\mathbf{a}_3, \qquad V_{\text{cell}} = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$$

Crystal = Bravais lattice + basis; atom positions $\mathbf{R} + \mathbf{r}_j$.

$$F_{\text{pack}} = \frac{N_{\text{atom}} V_{\text{atom}}}{V_{\text{cell}}}, \qquad V_{\text{atom}} = \frac{4\pi R^3}{3}.$$

(hkl) intercepts: $\mathbf{a}_1/h, \mathbf{a}_2/k, \mathbf{a}_3/l$. Cubic:

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

Reciprocal Lattice

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}, \qquad \mathbf{G}_{hkl} = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3$$

$$\mathbf{b}_1 = 2\pi\frac{\mathbf{a}_2 \times \mathbf{a}_3}{V_{\text{cell}}}, \quad \mathbf{b}_2 = 2\pi\frac{\mathbf{a}_3 \times \mathbf{a}_1}{V_{\text{cell}}}$$

$$\mathbf{b}_3 = 2\pi\frac{\mathbf{a}_1 \times \mathbf{a}_2}{V_{\text{cell}}}$$

$$d_{hkl} = 2\pi/|\mathbf{G}_{hkl}|.$$

Diffraction

$$\Delta\mathbf{k} = \mathbf{G}, \qquad \lambda = 2d_{hkl}\sin\theta$$

$$A(\mathbf{G}) \propto \sum_{\mathbf{R}} e^{i\mathbf{G}\cdot\mathbf{R}} \sum_j f_j e^{i\mathbf{G}\cdot\mathbf{r}_j} = L(\mathbf{G})S(\mathbf{G})$$

$$S(\mathbf{G}) = \sum_j f_j e^{i\mathbf{G}\cdot\mathbf{r}_j}, \qquad I \propto |S(\mathbf{G})|^2.$$

Insulators and Bands

Filled/empty bands carry no current. Odd electrons/unit cell imply a metal; even electrons may insulate if bands do not overlap.

Electrons and Holes

Hole = missing electron near a valence-band maximum.

$$E_h = -E, \qquad \mathbf{p}_h = -\hbar\mathbf{k}, \qquad q_h = +e, \qquad f_h = 1 - f$$

$$f_h(E_h) = \frac{1}{e^{(E_h+E_F)/(k_BT)} + 1} \quad (E_{F,h} = -E_F).$$

Near a valence-band top, holes have positive m^* and charge $+e$.

Parabolic Semiconductor Bands

$E_G = E_C - E_V$.

$$E_e = E_C + \frac{\hbar^2k^2}{2m_e}, \qquad E_h = -E_V + \frac{\hbar^2k^2}{2m_h}$$

$$g_e(E) = \frac{(2m_e)^{3/2}}{2\pi^2\hbar^3}\sqrt{E - E_C}, \quad g_h(E_h) = \frac{(2m_h)^{3/2}}{2\pi^2\hbar^3}\sqrt{E_h + E_V}.$$

Intrinsic Carriers

Boltzmann tails when E_F is far from band edges:

$$n_e = \int_{E_C}^{\infty} g_e(E)f(E)\,dE, \qquad n_h = \int_{-E_V}^{\infty} g_h(E_h)f_h(E_h)\,dE_h$$

$$n_e = N_C e^{-(E_C-E_F)/(k_BT)}$$

$$n_h = N_V e^{(E_V-E_F)/(k_BT)}$$

$$N_C = 2\left(\frac{2\pi m_e k_BT}{h^2}\right)^{3/2}$$

$$N_V = 2\left(\frac{2\pi m_h k_BT}{h^2}\right)^{3/2}$$

$$n_en_h = N_CN_V e^{-E_G/(k_BT)} \equiv n_i^2, \qquad n_i = \sqrt{N_CN_V}\,e^{-E_G/(2k_BT)}$$

Intrinsic: $n_e = n_h = n_i$.

$$E_F = \frac{E_C + E_V}{2} - \frac{3}{4}k_BT\ln(m_e/m_h).$$

E_F shifts toward the band with smaller effective DOS.

Conductivity

Electron and hole currents add:

$$j = -n_eev_e + n_hev_h, \qquad \sigma = \frac{n_ee^2\tau_e}{m_e} + \frac{n_he^2\tau_h}{m_h}$$

$$\sigma = n_ee\mu_e + n_he\mu_h, \qquad n_i \propto e^{-E_G/(2k_BT)}$$

$$E_G \simeq -2\,\frac{d\ln\sigma}{d(k_BT)^{-1}}.$$

Two-carrier Hall coefficient:

$$R_H = \frac{n_h\mu_h^2 - n_e\mu_e^2}{e(n_h\mu_h + n_e\mu_e)^2}.$$

Dopants

Group-V donors, group-III acceptors. Donor/acceptor levels:

$$g_D(E) = N_D\delta(E - E_D), \qquad g_A(E) = N_A\delta(E - E_A)$$

$$n_D = N_D\frac{1}{e^{(E_D-E_F)/(k_BT)} + 1}$$

$$n_A = N_A\frac{1}{e^{-(E_A-E_F)/(k_BT)} + 1}$$

Charge balance:

$$n_e - n_h + n_D - n_A = N_D - N_A.$$

Fully ionized shallow dopants: $n_D = n_A = 0$:

$$n_e - \frac{n_i^2}{n_e} = N_D - N_A.$$

Extrinsic Limits

If $|N_D - N_A| \gg n_i$ and $N_D > N_A$:

$$n_e \simeq N_D - N_A, \qquad n_h = \frac{n_i^2}{N_D - N_A}$$

$$E_F = E_C - k_BT\ln\left[\frac{N_C}{N_D - N_A}\right].$$

If $N_A > N_D$:

$$n_h \simeq N_A - N_D, \qquad n_e = \frac{n_i^2}{N_A - N_D}$$

$$E_F = E_V + k_BT\ln\left[\frac{N_V}{N_A - N_D}\right].$$

Decreasing T: intrinsic, extrinsic, freeze-out, zero-T. Intrinsic if $|N_D - N_A| \ll n_i$; extrinsic if $|N_D - N_A| \gg n_i$. Freeze-out: $k_BT \ll E_C - E_D$ for donors.

Hydrogenic Dopants

$$r_B^* = \frac{\epsilon m_e}{m_e^*}r_B, \qquad E_{\text{bind}} \simeq -\frac{m_e^*}{m_e\epsilon^2}R_E.$$

PN Junctions and Diodes

At equilibrium E_F is constant; band bending creates a depletion region.

$$I = I_0\left[\exp\left(\frac{eV}{k_BT}\right) - 1\right].$$

Forward bias: positive terminal to p side; reverse bias gives saturation current.

Optical Gaps

Direct gaps conserve crystal momentum; indirect gaps need phonons.