

Constantes

$$k_B = 1.381 \times 10^{-23} JK^{-1} = 8.26 \times 10^{-5} eVK^{-1}$$

$$m_e = 9.11 \times 10^{-31} kg = 0.511 MeVc^{-2}$$

$$\varepsilon_0 = \frac{1}{4\pi K} = 8.85 \times 10^{-12} Fm^{-1}$$

$$\hbar = 1.055 \times 10^{-34} Js = 6.58 \times 10^{-16} eVs$$

$$e = 1.602 \times 10^{-19} C$$

1 Estructura cristalina

1.1 Redes de Bravais

a	triclínica	P	Primitiva
m	monoclínica	S	Centrada en una cara
o	ortorrómbica	I	Centrada en el cuerpo
t	tetragonal	R	Centrada romboidal
h	hexagonal	F	Centrada en las caras
c	cúbica		

14 posibles redes de Bravais

Tric.	Monoc.	Ortor.	Tetra.	Hex.	Cúbico
aP	mP, mS	oP, oS, oF, oI	tP, tI	hP, hR	cP, cF, cI

1.2 Cosas

Base dual y matriz métrica

$$a^* = \frac{b \times c}{V}, \quad b^* = \frac{c \times a}{V}, \quad c^* = \frac{a \times b}{V}, \quad V = \det(\vec{a}, \vec{b}, \vec{c})$$

$$(\vec{a}^*, \vec{b}^*, \vec{c}^*) = \begin{pmatrix} \vec{a}^T \\ \vec{b}^T \\ \vec{c}^T \end{pmatrix}^{-1}, \quad G = \begin{pmatrix} a \cdot a & a \cdot b & a \cdot c \\ b \cdot a & b \cdot b & b \cdot c \\ c \cdot a & c \cdot b & c \cdot c \end{pmatrix}, \quad G^* = G^{-1}$$

Cambio de base

$$(\vec{a}', \vec{b}', \vec{c}') = (\vec{a}, \vec{b}, \vec{c})P, \quad \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix} = P^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

$$(x, y, z) = (x^*, y^*, z^*)P, \quad \begin{pmatrix} a'^* \\ b'^* \\ z'^* \end{pmatrix} = P^{-1} \begin{pmatrix} a^* \\ b^* \\ c^* \end{pmatrix}$$

Red recíproca y distancia interplanar $g_{hkl} = \frac{1}{d_{hkl}}$

Transferencia de momento $Q = \frac{4\pi \sin \theta}{\lambda}$

Condiciones de Laue $\vec{Q} = 2\pi \vec{g}_{hkl}$

Ley de Bragg $g_{hkl} = \frac{2 \sin \theta_{hkl}}{\lambda}$

Módulo de Young $\nu_s = \sqrt{\frac{2}{\rho}}$

Factor de estructura

$$F_{hkl} = \sum_p f_p e^{-i2\pi \vec{g}_{hkl} \cdot \vec{r}_p}, \quad I \propto |F_{hkl}|^2$$

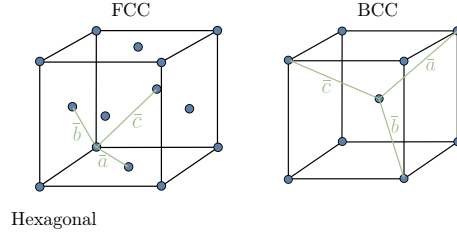
1.3 Estructuras comunes

FCC

$$\begin{cases} \vec{a} = \frac{1}{2}(1 \ 1 \ 0) \\ \vec{b} = \frac{1}{2}(0 \ 1 \ 1) \\ \vec{c} = \frac{1}{2}(1 \ 0 \ 1) \end{cases} \quad \begin{cases} \vec{a}^* = (1 \ 1 \ -1) \\ \vec{b}^* = (-1 \ 1 \ 1) \\ \vec{c}^* = (1 \ -1 \ 1) \end{cases}$$

BCC

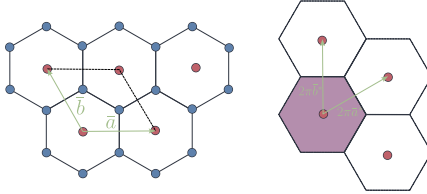
$$\begin{cases} \vec{a} = \frac{1}{2}(1 \ 1 \ -1) \\ \vec{b} = \frac{1}{2}(-1 \ 1 \ 1) \\ \vec{c} = \frac{1}{2}(1 \ -1 \ 1) \end{cases} \quad \begin{cases} \vec{a}^* = (1 \ 1 \ 0) \\ \vec{b}^* = (0 \ 1 \ 1) \\ \vec{c}^* = (1 \ 0 \ 1) \end{cases}$$



Hexagonal

$$\begin{cases} \vec{a} = (1, 0) \\ \vec{b} = (-\frac{1}{2}, \frac{\sqrt{3}}{2}) \end{cases} \quad \begin{cases} \vec{a}^* = \frac{2\sqrt{3}}{3}(\frac{\sqrt{3}}{2}, \frac{1}{2}) \\ \vec{b}^* = \frac{2\sqrt{3}}{3}(0, 1) \end{cases}$$

$$G = \begin{pmatrix} a^2 & -\frac{a^2}{2} & 0 \\ -\frac{a^2}{2} & a^2 & 0 \\ 0 & 0 & c^2 \end{pmatrix}, \quad G^* = \begin{pmatrix} \frac{4}{3a^2} & \frac{2}{3a^2} & 0 \\ \frac{2}{3a^2} & \frac{4}{3a^2} & 0 \\ 0 & 0 & \frac{1}{c^2} \end{pmatrix}$$



En una hcp $c = 1.633a$

1.4 Grupos

$$m_{100} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} n_{001} = \begin{pmatrix} \cos(\frac{360}{n}) & -\sin(\frac{360}{n}) & 0 \\ \sin(\frac{360}{n}) & \cos(\frac{360}{n}) & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Cambio de base a $\mathcal{B} = \{\vec{u}, \vec{v}, \vec{w}\}$

$$M_{\mathcal{C}} = M_{\mathcal{B} \rightarrow \mathcal{C}} M_{\mathcal{B}} M_{\mathcal{B} \rightarrow \mathcal{C}}^{-1}, \quad M_{\mathcal{B} \rightarrow \mathcal{C}} = (\vec{u}, \vec{v}, \vec{w})$$

Reflexión vector director (a, b, c)

$$M = \frac{1}{a^2 + b^2 + c^2} \begin{pmatrix} -a^2 + b^2 + c^2 & -2ab & -2ac \\ -2ab & a^2 - b^2 + c^2 & -2bc \\ -2ac & -2bc & a^2 + b^2 - c^2 \end{pmatrix}$$

Rotación respecto $\hat{u} = (u_x, u_y, u_z)$ ($c = \cos \theta$, $s = \sin \theta$).

$$R = \begin{pmatrix} c + u_x^2(1-c) & u_x u_y(1-c) - u_z s & u_x u_z(1-c) + u_y s \\ u_y u_x(1-c) + u_z s & c + u_y^2(1-c) & u_y u_z(1-c) - u_x s \\ u_z u_x(1-c) - u_y s & u_z u_y(1-c) + u_x s & c + u_z^2(1-c) \end{pmatrix}$$

Centrosimétricos $(x, y, z) \rightarrow (-x, -y, -z)$ no tienen polarización espontánea

2 Dinámica de cristales

2.1 Densidad de estados

$$\vec{k} = \left(\frac{2\pi}{L} n \quad \frac{2\pi}{L} m \quad \frac{2\pi}{L} l \right) \quad \forall n, m, l \in \mathbb{Z}$$

Número de estados hasta k

$$N(k) = \int_{(\frac{2\pi}{L})^2(n^2+m^2+l^2) \leq k^2} dV = \frac{L^3}{6\pi^2} k^3 = \frac{V}{6\pi^2} k^3$$

1, 2 y 3 dimensiones respectivamente (y se cumple $\omega = \nu_s k$)

$$\begin{cases} g(k) = \frac{L}{\pi} & \begin{cases} g(k) = \frac{L^2}{2\pi} k \\ g(\omega) = \frac{L}{\pi \nu} \end{cases} & \begin{cases} g(k) = \frac{V}{2\pi^2} k^2 \\ g(\omega) = \frac{V}{2\pi^2 \nu_s^3} \omega^2 \end{cases} \end{cases}$$

2.2 Dispersión

Oscilador con masa m y constante k_s

$$F_n = m\ddot{x}_n = k_s(x_{n+1} + x_{n-1} - 2x_n)$$

$$-m\omega^2 A e^{i(kna - \omega t)} = k_s A e^{i(kna - \omega t)} (e^{ika} + e^{-ika} - 2) =$$

$$= -4k_s \sin^2\left(\frac{ka}{2}\right) \Rightarrow \left| \omega = 2\sqrt{\frac{k_s}{m}} \sin\left(\frac{ka}{2}\right) \right|$$

Oscilador con masa m y constantes alternadas k_1, k_2

$$\begin{cases} m\ddot{x}_n = k_1(y_{n-1} - x_n) + k_2(y_n - x_n) \\ m\ddot{y}_n = k_1(x_{n+1} - y_n) + k_2(x_n - y_n) \end{cases}$$

Ansatz

$$x_n = A e^{i(kna - \omega t)} \quad y_n = B e^{i(kna - \omega t)}$$

Ecuaciones

$$\begin{cases} -m\omega^2 A = -A(k_1 + k_2) + B(k_1 e^{ika} + k_2) \\ -m\omega^2 B = -A(k_1 e^{ika} + k_2) + B(-k_1 - k_2) \end{cases}$$

Forma matricial

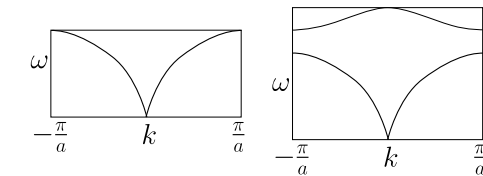
$$m\omega^2 \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} (k_1 + k_2) & -k_2 - k_1 e^{ika} \\ -k_2 - k_1 e^{ika} & (k_1 + k_2) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = K \begin{pmatrix} A \\ B \end{pmatrix}$$

$$0 = \det(K - m\omega^2 I) = |(k_1 + k_2) - m\omega^2|^2 - |k_2 + k_1 e^{ika}|^2$$

$$\omega_{\pm}(k) = \sqrt{\frac{k_1 + k_2}{m} \pm \frac{1}{m} \sqrt{(k_1 + k_2)^2 - 4k_1 k_2 \sin^2(ka/2)}}$$

Si $m_1 \neq m_2$ y k_s es la misma, sea $K_i = \frac{k}{m_i}$, entonces

$$\omega_{\pm}(k) = \sqrt{(K_1 + K_2) \pm \sqrt{(K_1 + K_2)^2 - 4K_1 K_2 \sin^2(ka/2)}}$$



2.3 Modelo de Einstein

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right) \Rightarrow Z_1 = \frac{1}{2 \sinh\left(\frac{\beta \hbar \omega}{2}\right)}$$

$$\langle E_1 \rangle = -\frac{\partial}{\partial \beta} \ln Z_1 = \frac{\hbar\omega}{2} \coth\left(\frac{\beta \hbar \omega}{2}\right)$$

Energía y capacidad calorífica

$$\langle E \rangle = \frac{3}{2} N \hbar \omega \coth\left(\frac{\beta \hbar \omega}{2}\right)$$

$$C_v = \frac{\partial \langle E \rangle}{\partial T} = 3Nk_B (\beta \hbar \omega)^2 \frac{e^{\beta \hbar \omega}}{(e^{\beta \hbar \omega} - 1)^2}$$

Definimos ahora $T_E = \frac{\hbar \omega_E}{k_B}$. En los límites

- Si $T \gg T_E \Rightarrow C_v = 3Nk_B$
- Si $T \ll T_E \Rightarrow C_v = 3Nk_B \left(\frac{T_E}{T}\right)^2 \frac{1}{\sinh^2\left(\frac{T_E}{2T}\right)}$

2.4 Modelo de Debye

Aproximamos la ecuación de dispersión para k baja como $\omega = \nu k$

$$3N = \int_0^{\omega_D} 3g(\omega) d\omega = \frac{V}{2\pi^2 \nu^3} \omega_D^3 \Rightarrow \omega_D = \sqrt[3]{\frac{6\pi^2 \nu^3 N}{V}}$$

donde hemos contado cada partícula y cada estado 3 veces y hemos usado

$$\omega = \nu k, \quad g(k) = \frac{V}{2\pi^2} k^2, \quad g(\omega) = \frac{V}{2\pi^2 \nu^3} \omega^2$$

La energía y la capacidad calorífica

$$\langle E \rangle = \int_0^{\omega_D} \hbar \omega 3g(\omega) \left(\frac{1}{e^{\beta \hbar \omega} - 1} + \frac{1}{2} \right) d\omega =$$

$$= E_0 + \frac{3V\hbar}{2\pi^2 \nu^3} \int_0^{\omega_D} \frac{\hbar \omega^3}{e^{\beta \hbar \omega} - 1} d\omega \quad (x = \frac{\hbar \omega}{k_B T})$$

$$T_D := \frac{\hbar \omega}{k_B} \Rightarrow \langle E \rangle = \frac{3V k_B^4 T^4}{2\pi^2 \nu^3 \hbar^3} \int_0^{\frac{T_D}{T}} \frac{x^3}{e^x - 1} dx$$

La capacidad calorífica $C_v = \frac{\partial \langle E \rangle}{\partial T}$ en los extremos:

- Si $T \gg T_D \Rightarrow \langle E \rangle \sim 3Nk_B T \Rightarrow C_v \sim 3Nk_B$
- Si $T \ll T_D \Rightarrow \langle E \rangle \sim \frac{3\pi^4 N k_B T^4}{5T_D^4} \Rightarrow C_v \sim \frac{12\pi^4}{5} N k_B \left(\frac{T}{T_D}\right)^3$

3 No se, cuanticocosas

3.1 Drude model

$$n = \frac{N}{V}; \quad \frac{dp}{dt} = F - \frac{p}{\tau}, \quad \vec{j} = -ne\vec{v} = \sigma\vec{E}$$

$$mv = p = -e\tau E; \quad R_H = \frac{-1}{ne} = \frac{\rho_{yx}}{|B|}$$

$$\vec{E} = \bar{\rho}\vec{j}; \quad \rho_{xx} = \rho_{yy} = \rho_{zz} = \frac{m}{ne^2\tau}$$

$$\text{Hall resistivity } \rho_{xy} = -\rho_{yx} = \frac{B}{ne} (\vec{B} \propto \hat{z})$$

$$\text{Peltier coefficient } \Pi = -\frac{k_B T}{2e} = -\frac{c_v T}{3e}$$

$$\text{Seebeck coefficient } S = \frac{\Pi}{T}$$

$$\langle v \rangle_{\text{gasid.}} = \sqrt{\frac{8k_B T}{\pi m}}; \quad \kappa = \frac{1}{3}nc \langle v \rangle^2 \tau = \frac{4}{\pi} \frac{n\tau k_B^2 T}{m}$$

3.2 Capacidad calorífica

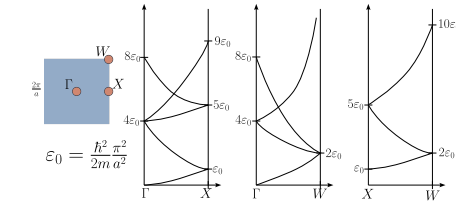
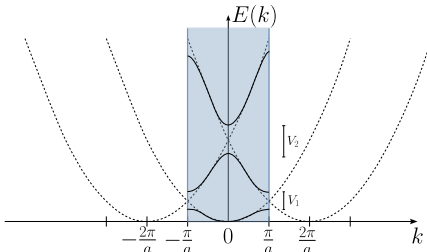
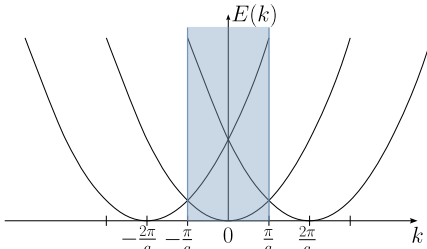
g densidad de estados / V

$$g(\varepsilon) = \frac{3n}{2(E_F)^{\frac{3}{2}}} \varepsilon^{\frac{1}{2}} = \frac{(2m)^{\frac{3}{2}}}{2\pi^2 \hbar^3} \varepsilon^{\frac{1}{2}}, \quad k = \sqrt{\frac{2\varepsilon m}{\hbar^2}}$$

$$N = \int_0^\infty d\varepsilon g(\varepsilon) n_F(\beta(\varepsilon - \mu)), \quad E_T = \int_0^\infty d\varepsilon \varepsilon g(\varepsilon) n_F(\beta(\varepsilon - \mu))$$

$$C = \frac{\pi^2}{3} \left(\frac{3Nk_B}{2} \right) \left(\frac{T}{T_F} \right)$$

$$\overline{M} = g(E_F) \mu_B^2 \overline{B}; \quad \mu_B = 0.67 \left(\frac{K}{\text{Tesla}} \right) k_B$$



Teorema de Bloch ($V(\vec{r})$ periódico)

$$\psi_{\vec{k}}(\vec{r}) = u_{\vec{k}}(\vec{r}) e^{i\vec{k} \cdot \vec{r}}, \quad E(\vec{k}) = E(\vec{k} + \vec{G})$$

(1D) Fourier del potencial de dos formas

$$V(x) = V_0 + \sum_{j=1}^{\infty} V_j \cos\left(\frac{2\pi j}{a} x\right) \quad \text{ó} \quad V(x) = \sum_{j=-\infty}^{\infty} V_{\frac{2\pi j}{a}} e^{i\frac{2\pi j}{a} x}$$

Con las relaciones $V_j = 2V_{\frac{2\pi j}{a}}$, y donde los coeficientes son

$$V_j = \frac{2}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx V(x) \cos\left(\frac{2\pi j}{a} x\right); \quad V_{\frac{2\pi j}{a}} = \frac{1}{a} \int_{-\frac{a}{2}}^{\frac{a}{2}} dx V(x) e^{-i\frac{2\pi j}{a} x}$$

Gas de electrones libres

$$\vec{k} = \frac{2\pi}{L}(n_x, n_y, n_z), \quad E(\vec{k}) = \frac{\hbar^2}{2m} |\vec{k}|^2, \quad n_F(x) = \frac{1}{e^x + 1}$$

$$N = 2 \sum_{\vec{k}} n_F(\beta(E(\vec{k}) - \mu)) = 2 \frac{V}{(2\pi)^3} \int d\vec{k} n_F(\beta(E(\vec{k}) - \mu))$$

Fermi energy ($E_F = \mu(T \rightarrow 0)$)

$$E_F = \frac{\hbar^2 k_F^2}{2m} = k_B T_F, \quad p_F = \hbar k_F$$

$$N = 2 \frac{V}{(2\pi)^3} \int_{|k| < k_F} dk \Rightarrow k_F = (3\pi^2 n)^{\frac{1}{3}}, \quad E_F = \frac{\hbar^2 (3\pi^2 n)^{\frac{2}{3}}}{2m}$$

$$\vec{k} = \frac{2\pi}{L} \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix}, \quad n_x, n_y, n_z \in \mathbb{Z} \Rightarrow k^2 = \left(\frac{2\pi}{L}\right)^2 (n_x^2 + n_y^2 + n_z^2)$$

Considerando los dos espines (multiplicamos por 2)

$$N_T = 2 \cdot \left(\frac{4}{3} \pi (n_x^2 + n_y^2 + n_z^2)^{3/2} \right) \Rightarrow k_{max}^2 = k_F^2 = (3n\pi^2)^{\frac{2}{3}}$$

Electrones casi-libres

$$\psi_+ \sim \cos(\pi \frac{x}{a}), \quad \psi_- \sim \sin(\pi \frac{x}{a})$$

$$E^{\pm} = \frac{1}{2} (E_{\vec{k}-\vec{G}}^0 + E_{\vec{k}}^0) \pm \sqrt{\frac{1}{4} (E_{\vec{k}-\vec{G}}^0 - E_{\vec{k}}^0)^2 + |V_{\vec{G}}|^2}$$

Enlace fuerte, celda primitiva cúbica

$$E(\vec{k}) \approx E_i - A - 2B(\cos k_x a + \cos k_y a + \cos k_z a)$$

$$A = -\langle \varphi_{i,n} | v | \varphi_{i,n} \rangle, \quad B = -\langle \varphi_{i,m} | v | \varphi_{i,n} \rangle$$

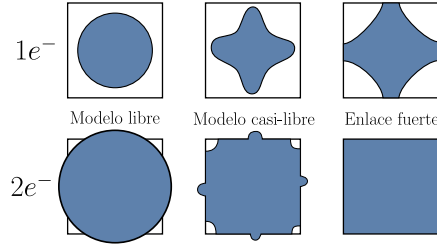
$$\vec{v} = \nabla_{\vec{k}} \omega(\vec{k}) = \frac{1}{\hbar} \nabla_{\vec{k}} E(\vec{k})$$

Carga de un campo $\vec{\mathcal{E}}$

$$\dot{v}_i = \frac{1}{\hbar^2} \sum_j \frac{\partial^2 E}{\partial k_i \partial k_j} (-e \mathcal{E}_j), \quad \left(\frac{1}{m^*} \right)_{ij} = \frac{1}{\hbar^2} \frac{\partial^2 E(\vec{k})}{\partial k_i \partial k_j}$$

Caso totalmente degenerado

$$m^* = \frac{\hbar^2}{\left(\frac{d^2 E}{dk^2} \right)}, \quad E(\vec{k}) = E_0 + \frac{\hbar^2}{2m^*} |k|^2, \quad \sigma \simeq \frac{e^2 \tau (E_F) n}{m^*}$$

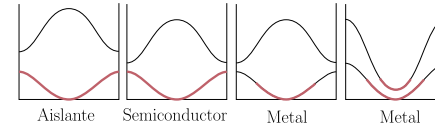


Tipos de materiales

Aislante: Banda llena ($2e^-$). $V_g > 4eV$

Semiconductor Banda llena ($2e^-$). $V_g < 4eV$.

Metal Banda semillena ($1e^-$ ó $2e^-$ con bandas solapantes).



4 Semiconductores

Densidad de estados

$$D_C = \frac{(2m_n^*)^{2/3}}{2\pi^2 \hbar^3} \sqrt{E - E_C}, \quad D_V = \frac{(2m_p^*)^{2/3}}{2\pi^2 \hbar^3} \sqrt{E_V - E}$$

$$n = 2 \left(\frac{2\pi m_n^* k_B T}{\hbar^2} \right)^{3/2} e^{\beta(E_F - E_C)} = N_{eff}^C e^{\beta(E_F - E_C)}$$

$$p = 2 \left(\frac{2\pi m_p^* k_B T}{\hbar^2} \right)^{3/2} e^{\beta(E_V - E_F)} = N_{eff}^V e^{\beta(E_V - E_F)}$$

$$np = N_{eff}^C N_{eff}^V e^{-\beta E_g} = 4 \left(\frac{k_B T}{2\pi \hbar^2} \right)^3 (m_n^* m_p^*)^{3/2} e^{-\beta E_g}$$

$$e^{\beta E_F} = \frac{N_{eff}^V}{N_{eff}^C} e^{\beta(E_V + E_C)}, \quad E_F = \frac{E_C + E_V}{2} + \frac{3}{4} k_B T \ln \left(\frac{m_p^*}{m_n^*} \right)$$

$$\mu = \frac{e\tau}{m^*}, \quad \sigma = e(n\mu_n + p\mu_p), \quad E_g = E_C - E_V$$

Semiconductores dopados

$$E_n = \frac{m^* e^4}{2(4\pi\epsilon\hbar)^2} \frac{1}{n^2}, \quad r = \epsilon \frac{\hbar^2}{\pi m^* e^2}$$

$$n \approx \frac{2N_D}{1 + \sqrt{1 + 4 \frac{N_D}{N_{eff}^C} e^{\beta E_d}}}$$

Unión p-n

$$n_n = N_{eff}^C e^{\beta(E_F - E_n^0)}; \quad p_p = N_{eff}^V e^{\beta(E_V - E_F)}$$

$$d_n^0 = \sqrt{\frac{2\epsilon V_D}{e} \frac{N_A/N_D}{N_A + N_D}}; \quad d_p^0 = \sqrt{\frac{2\epsilon V_D}{e} \frac{N_D/N_A}{N_A + N_D}}$$

$$d_n(U) = d_n^0 \sqrt{1 - \frac{U}{V_D}}; \quad d_p(U) = d_p^0 \sqrt{1 - \frac{U}{V_D}}$$

$$eV_D = k_B T \ln \left(\frac{n_n p_p}{n_i^2} \right); \quad I(U) = (I_n^{gen} + I_p^{gen})(e^{\beta eU} - 1)$$

5 Mates

$$\sin^2 \left(\frac{x}{2} \right) = \frac{1 - \cos a}{2}$$

$$\int_0^\infty \frac{1}{e^x - 1} dx = +\infty, \quad \int_0^\infty \frac{1}{e^x + 1} dx = \ln(2)$$

$$\int_0^\infty \frac{x}{e^x - 1} dx = \frac{\pi^2}{6}, \quad \int_0^\infty \frac{x}{e^x + 1} dx = \frac{\pi^2}{12}$$

$$\int_0^\infty \frac{x^2}{e^x - 1} dx = 2\zeta(3), \quad \int_0^\infty \frac{x^2}{e^x + 1} dx = \frac{3}{2}\zeta(3)$$

$$\int_0^\infty \frac{x^3}{e^x - 1} dx = \frac{\pi^4}{15}, \quad \int_0^\infty \frac{x^3}{e^x + 1} dx = \frac{7\pi^4}{120}$$