

Formula page

1. LATTICES

Reciprocal lattice \mathbf{G} is defined by $e^{i\mathbf{G}\cdot\mathbf{R}} = 1$ with \mathbf{R} the lattice vector.

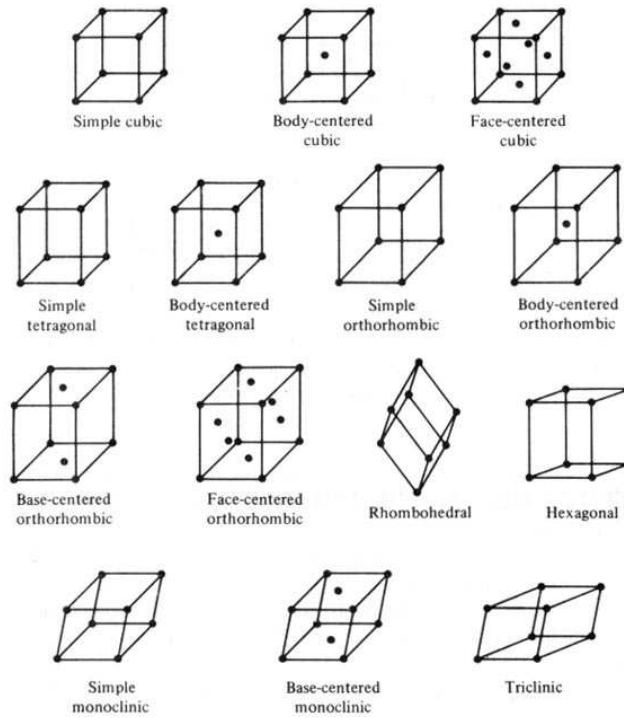
\mathbf{a}_i is the primitive direct lattice vector $\mathbf{R} = \sum_i^d \mathbf{a}_i n_i$, d is the dimension, $n_i \in \mathbb{Z}$.

\mathbf{b}_i is the primitive reciprocal lattice vector $\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$, or

$$\mathbf{b}_1 = 2\pi \frac{\mathbf{a}_2 \times \mathbf{a}_3}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \quad \mathbf{b}_2 = 2\pi \frac{\mathbf{a}_3 \times \mathbf{a}_1}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)} \quad \mathbf{b}_3 = 2\pi \frac{\mathbf{a}_1 \times \mathbf{a}_2}{\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)}$$

The primitive cell volume $V = |\mathbf{a}_1 \cdot (\mathbf{a}_2 \times \mathbf{a}_3)|$.

Three dimensional Bravais Lattices:



2. DIFFRACTION

Bragg condition $|\mathbf{G}| = 2|\mathbf{k}|\sin(\phi/2)$, with $\mathbf{k} = \frac{2\pi}{\lambda}\hat{\mathbf{k}}$ the incident wave and λ the wavelength. $\cos(\phi) = \hat{\mathbf{k}} \cdot \hat{\mathbf{k}}_{out}$

The structure factor $S_{\mathbf{G}} = \sum_i f_i e^{i\mathbf{G}\cdot\mathbf{d}_i}$, with \mathbf{d}_i the basis vectors, $f_i(\mathbf{G})$ the atomic form factor $f_i(\mathbf{G}) = -\frac{1}{e} \int_{\mathbf{r}} \rho_i(\mathbf{r}) e^{i\mathbf{G}\cdot\mathbf{r}}$. The intensity is $I \sim |S_{\mathbf{G}}|^2$.

3. COHESIVE ENERGY

Lennard Jones potential

$$u = 2\epsilon \left[A_{12} \left(\frac{\sigma}{r} \right)^{12} + A_6 \left(\frac{\sigma}{r} \right)^6 \right]$$

$$A_n = \sum_{\mathbf{R} \neq 0} \frac{1}{|\mathbf{R}|^n}$$

Coulomb energy $u = -\frac{e^2}{d}\alpha$, $\alpha = \sum_j \frac{(-1)^j}{|r_j/d|}$.

4. PHONONS

The Harmonic energy with potential $\phi(\mathbf{r})$

$$U^{Harmonic} = \frac{1}{2} \sum_{\mathbf{R}_1, \mathbf{R}_2} \sum_{\mu, \nu = x, y, z} [u_\mu(\mathbf{R}_1) - u_\mu(\mathbf{R}_2)] \frac{\partial^2 \phi(\mathbf{r})}{\partial r_\mu \partial r_\nu} [u_\nu(\mathbf{R}_1) - u_\nu(\mathbf{R}_2)]$$

The equations of motions are $m\ddot{\mathbf{u}}(\mathbf{R}) = -\frac{\partial U}{\partial \mathbf{u}(\mathbf{R})}$, with periodic boundary conditions we seek solution of the form $\mathbf{u} = \boldsymbol{\epsilon} e^{i\mathbf{k} \cdot \mathbf{R} - i\omega t}$, $\boldsymbol{\epsilon}$ the polarization vector.

In k space the dynamical matrix $\ddot{D}(\mathbf{k})\boldsymbol{\epsilon} = M\omega^2\boldsymbol{\epsilon}$. For oscillation in d dimensions of p atoms in a unit cell, there are d acoustic branches and $(p-1)d$ optical branches.

The vibrational energy and specific heat for each branch:

$$\frac{U}{V} = \sum_s \int_{\omega} g_s(\omega) f(\omega) \hbar \omega d\omega = \sum_s \int_{FBZ} \frac{d\mathbf{k}}{(2\pi)^3} f(\omega_s(\mathbf{k})) \hbar \omega_s(\mathbf{k})$$

$$c_V = \frac{1}{V} \frac{dU}{dT}$$

$$f(\omega) = \frac{1}{e^{\beta \hbar \omega_s(\mathbf{k})} - 1}$$

$$g_s(\omega) = \frac{dn_s}{d\omega}$$

(density of states per unit volume for branch s)

$$\Delta k = (2\pi)^d / V$$

(density in k -space)

5. ELECTRONS

The Drude conductivity is $\sigma = ne^2\tau/m$, with n the number of electron per unit volume, and τ the mean free time. The equation of motion for the momentum in Drude theory is

$$\frac{d\mathbf{p}}{dt} = -e \left(\mathbf{E} + \frac{\mathbf{p}}{mc} \times \mathbf{H} \right) - \frac{\mathbf{p}}{\tau}$$

The cyclotron frequency is $\omega_c = \frac{eH}{mc}$, the plasma frequency is $\omega_p^2 = \frac{4\pi n e^2}{m}$ the current density is $\mathbf{j} = \frac{ne}{m}\mathbf{p}$, and the conductivity tensor σ is defined by $\mathbf{j} = \sigma \mathbf{E}$.

The occupation functions are

$$f(\epsilon) = \begin{cases} \frac{1}{e^{\beta(\epsilon-\mu)} + 1} & \text{Fermi-Dirac} \\ \frac{1}{e^{\beta(\epsilon-\mu)} - 1} & \text{Bose-Einstein} \end{cases}$$

Fermi surface $\epsilon(\mathbf{k}) = \epsilon_F$. Sommerfeld expansions are

$$\begin{aligned} \int_{-\infty}^{\infty} H(x)f(x)dx &= \int_{-\infty}^{\mu} H(x)dx + \frac{\pi^2}{6}(k_B T)^2 H'(\mu) + \frac{7\pi^4}{360}(k_B T)^4 H'''(\mu) + \dots \\ \mu &= \epsilon_F - \frac{\pi^2}{6} \frac{g'(\epsilon_F)}{g(\epsilon_F)} (k_B T)^2 \\ u &= u_0 + \frac{\pi^2}{6} g(\epsilon_F) (k_B T)^2 \end{aligned}$$

The specific heat of electron gas in low temperature is $c_v = \frac{\partial u}{\partial T} = \frac{\pi^2}{3} k_B^2 T g(\epsilon_F)$, where the density of states is $g(\epsilon) = \frac{\partial n(\epsilon)}{\partial \epsilon}$.

Bloch theorem $\psi(\mathbf{r} + \mathbf{R}) = e^{i\mathbf{k}\cdot\mathbf{R}}\psi(\mathbf{r})$, electron velocity in energy $E_n(\mathbf{k})$: $\mathbf{v}_n(\mathbf{k}) = \frac{1}{\hbar}\nabla_{\mathbf{k}}E_n(\mathbf{k})$.

Effective mass tensor

$$\frac{1}{m_{i,j}^*} = \frac{1}{\hbar^2} \frac{\partial^2 \epsilon(\mathbf{k})}{\partial k_i \partial k_j} \quad i, j = x, y, z$$

Therefore, $m^* \frac{d\mathbf{v}}{dt} = \hbar \frac{d\mathbf{k}}{dt}$

Electron \mathbf{k} in a periodic potential

$$\epsilon_{\mathbf{k}-\mathbf{G}}^0 c_{\mathbf{k}-\mathbf{G}} + \sum_{\mathbf{G}'} U_{\mathbf{G}'-\mathbf{G}} c_{\mathbf{k}-\mathbf{G}'} = \epsilon_{\mathbf{k}-\mathbf{G}} c_{\mathbf{k}-\mathbf{G}}$$

where $U_{\mathbf{G}} = \frac{1}{v_{p.u.c}} \int_{p.u.c} U(\mathbf{r}) e^{-i\mathbf{G}\cdot\mathbf{r}} d\mathbf{r}$ are the Fourier components of the potential, *p.u.c* = primitive unit cell. the $c_{\mathbf{k}-\mathbf{G}}$ are the Fourier components of the wave function and $\epsilon_{\mathbf{k}-\mathbf{G}}^0 = \frac{\hbar^2}{2m}(\mathbf{k} - \mathbf{G})^2$ is the free electron energy.

For a weak potential, near a couple of degenerate states

$$\epsilon = \frac{1}{2}(\epsilon_{\mathbf{k}}^0 + \epsilon_{\mathbf{k}-\mathbf{G}}^0) \pm \left[\left(\frac{\epsilon_{\mathbf{k}}^0 - \epsilon_{\mathbf{k}-\mathbf{G}}^0}{2} \right)^2 + |U_{\mathbf{G}}|^2 \right]^{1/2}$$

Far from degenerate states

$$\epsilon_{\mathbf{k}} = \epsilon_{\mathbf{k}}^0 + \sum_{\mathbf{G}} \frac{|U_{\mathbf{G}}|^2}{\epsilon_{\mathbf{k}}^0 - \epsilon_{\mathbf{k}-\mathbf{G}}^0}$$

Tight Binding model

$$\epsilon(\mathbf{k}) = E_s - \beta - \sum_{\mathbf{R}} \gamma(\mathbf{R}) \cos(\mathbf{k} \cdot \mathbf{R})$$

where E_s is the energy of atomic s-level, and

$$\beta = - \int d\mathbf{r} \Delta U(\mathbf{r}) |\phi(\mathbf{r})|^2$$

$$\gamma(\mathbf{R}) = - \int d\mathbf{r} \phi^*(\mathbf{r}) \Delta U(\mathbf{r}) \phi(\mathbf{r} - \mathbf{R})$$

6. CONSTANTS, INTEGRALS, MISC

Constants:

$$\hbar = 1.054 \cdot 10^{-34} \text{ [J s]}$$

$$k_B = 1.38 \cdot 10^{-23} \text{ [J/K]}$$

$$N_A = 6.022 \cdot 10^{23} \text{ [1/mole]}$$

$$m_e = 9.11 \cdot 10^{-31} \text{ [kg]}$$

$$e = 1.6 \cdot 10^{-19} \text{ [C]}$$

Integrals:

$$\int_0^\infty \frac{x^4 e^x}{(e^x - 1)^2} dx = \frac{4\pi^2}{15}$$

$$\int_0^1 \frac{x^4 e^x}{(e^x - 1)^2} dx \approx 0.32$$

$$\lim_{A \rightarrow 0} \int_0^A \frac{x^4 e^x}{(e^x - 1)^2} dx = \frac{A^3}{3}$$

$$\int_0^\infty \frac{x^3 e^x}{(e^x - 1)^2} dx = 6\zeta(3) \approx 7.2$$

$$\int_0^\infty \frac{x^4 e^x}{(e^x + 1)^2} dx = \frac{7\pi^4}{30}$$

$$\int_0^1 \frac{x^4 e^x}{(e^x + 1)^2} dx \approx 0.042$$

$$\lim_{A \rightarrow 0} \int_0^A \frac{x^4 e^x}{(e^x + 1)^2} dx = \frac{A^5}{20}$$

Ellipse equation and its area:

$$\left(\frac{x}{a}\right)^2 + \left(\frac{y}{b}\right)^2 = 1 \quad , \quad A = \pi ab$$

Trigonometric identities:

$$\sin(2\theta) = 2 \sin(\theta) \cos(\theta)$$

$$\cos(2\theta) = 2 \cos^2(\theta) - 1$$