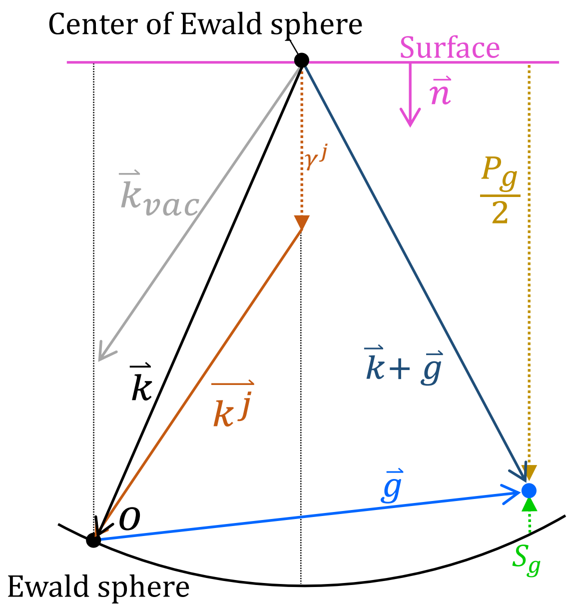
Definitions of vectors and scalars



$\longrightarrow$ Vector

$\dashrightarrow$ Scalar

$\vec{n}$: Unit vector normal to surface

$$P_g = 2\vec{n}(\vec{k}+\vec{g})$$

$$Q_g = |\vec{k}|^2 - |\vec{k}+\vec{g}|^2 = -\vec{g}(2\vec{k}+\vec{g})$$

$$S_g = \frac{\sqrt{{P_g}^2 + 4Q_g} - P_g}{2}$$

$$R = |\vec{g}|^2 |Q_g|$$

(Evaluation function)

Schrödinger's equation

$$\nabla^2 \Psi(\mathbf{r}) + 4\pi^2 \left\{ {k_{vac}}^2 + \sum_g U_g e^{2\pi i \mathbf{g}\cdot\mathbf{r}} \right\} \Psi(\mathbf{r}) = 0$$

k_{vac}: Wavenumber of electron in vacuum
U_g: Fourier component of potential

Bloch's theorem

$$\Psi(\mathbf{r}) = b\left(\mathbf{k}^{(j)}, \boldsymbol{r}\right) = u(\mathbf{r}) \exp(2\pi i \mathbf{k}^{(j)} \cdot \mathbf{r})$$

$u(\mathbf{r})$: Periodic function with the same periodicity as the crystal lattice
$\mathbf{k}^{(j)}$: j^{th} Bloch wave vector

Bethe's dynamical equation

$$\left[k^2 - \left(\mathbf{k}^{(j)} + \mathbf{g}\right)^2 + i\,U'_{g,g}\right] C_g^{(j)} + \sum_{h \neq g} \left(U_{g-h} + i\,U'_{g,h}\right) C_h^{(j)} = 0$$

Eigen values/vectors equation

$$\begin{pmatrix} (Q_0 + iU'_{0,0})/P_0 & (U_{-g} + iU'_{0,g})/P_0 & (U_{-h} + iU'_{0,h})/P_0 & \cdots \\ (U_g + iU'_{g,0})/P_g & (Q_g + iU'_{g,g})/P_g & (U_{g-h} + iU'_{g,h})/P_g & \cdots \\ (U_h + iU'_{h,0})/P_h & (U_{h-g} + iU'_{h,g})/P_h & (Q_h + iU'_{h,h})/P_h & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_0^{(1)} & C_0^{(2)} & C_0^{(3)} & \cdots \\ C_g^{(1)} & C_g^{(2)} & C_g^{(3)} & \cdots \\ C_h^{(1)} & C_h^{(2)} & C_h^{(3)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$= \begin{pmatrix} C_0^{(1)} & C_0^{(2)} & C_0^{(3)} & \cdots \\ C_g^{(1)} & C_g^{(2)} & C_g^{(3)} & \cdots \\ C_h^{(1)} & C_h^{(2)} & C_h^{(3)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \lambda^{(1)} & 0 & 0 & \cdots \\ 0 & \lambda^{(2)} & 0 & \cdots \\ 0 & 0 & \lambda^{(3)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

U_g: Crystal potential for elastic scattering
U'_g: Imaginary (absorption) potential for thermal diffuse scattering
$P,\ Q$: Defined in above figure
$\lambda^{(j)}$: j^{th} eigen value
$C_*^{(j)}$: j^{th} eigen vectors

Optical potential (complex crystal potential)

注: ReciProのDetailsで表示されるテーブル中の U_g は、相対論補正項γを掛ける前の数値.

Crystal potential for elastic scattering

$$U_g = \gamma \frac{1}{\pi\,\Omega} \sum_k f_k(\mathbf{g}) \exp[2\pi i\ \mathbf{g}\cdot\mathbf{r_k}]\, T_k(\mathbf{g}, M_k)$$

$$f_k(\mathbf{g}) = \textstyle\sum_i a_i \exp[-b_i\,|\mathbf{g}|^2/4]$$

$$T_k(\mathbf{g}, M_k) = \exp[-M_k\,|\mathbf{g}|^2/4]$$

Imaginary (absorption) potential for thermal diffuse

$$U'_{g,h} = \gamma \frac{1}{\pi\,\Omega} \sum_k f_k{}'(\mathbf{g},\mathbf{h}) \exp[2\pi i(\mathbf{g}-\mathbf{h})\cdot\mathbf{r_k}]\, T_k(\mathbf{g}-\mathbf{h}, M_k)$$

$$f'_k(\mathbf{g},\mathbf{h}) = \frac{2\,h}{\beta\, m_0\, c} \sum_i \sum_j a_i a_j \left(\frac{\exp\left\{-\frac{b_i b_j}{b_i+b_j}\frac{|\mathbf{g}-\mathbf{h}|^2}{4}\right\}}{b_i+b_j} - \frac{\exp\left\{-\frac{b_i b_j - M_k{}^2}{b_i+b_j+2M_k}\frac{|\mathbf{g}-\mathbf{h}|^2}{4}\right\}}{b_i+b_j+2M_k} \right)$$

Ω: Unit cell volume
$\gamma = m/m_0 = 1 + (e_0 E)/(m_0\, c^2)$
$\beta = v/c = \sqrt{1-(m_0/m)^2} = \sqrt{1-\gamma^{-2}}$

Debye-Waller factor

$$T_k(\mathbf{g}) = \exp[-2\pi\ \mathbf{g}^{\mathrm{t}}\ \mathbf{U}\ \mathbf{g}]$$

$$\begin{aligned}\mathbf{g}^{\mathrm{t}}\,\mathbf{U}\,\mathbf{g} &= \begin{pmatrix} g_x & g_y & g_z \end{pmatrix} \begin{pmatrix} U_{11} & U_{12} & U_{13} \\ U_{12} & U_{22} & U_{23} \\ U_{13} & U_{23} & U_{33} \end{pmatrix} \begin{pmatrix} g_x \\ g_y \\ g_z \end{pmatrix} \\ &= g_x^2 U_{11} + g_y^2 U_{22} + g_z^2 U_{33} + 2\left(g_x g_y U_{12} + g_y g_z U_{23} + g_x g_z U_{13}\right)\end{aligned}$$

$$\begin{pmatrix} g_x \\ g_y \\ g_z \end{pmatrix} = \begin{pmatrix} a_x^* & b_x^* & c_x^* \\ a_y^* & b_y^* & c_y^* \\ a_z^* & b_z^* & c_z^* \end{pmatrix} \begin{pmatrix} h \\ k \\ l \end{pmatrix} = \begin{pmatrix} h\,a_x^* + k\,b_x^* + l\,c_x^* \\ h\,a_y^* + k\,b_y^* + l\,c_y^* \\ h\,a_z^* + k\,b_z^* + l\,c_z^* \end{pmatrix}$$

Matrix representation of transmission coefficient T_g

$$\begin{pmatrix} T_0 \\ T_g \\ T_h \\ \vdots \end{pmatrix} = e^{-2\pi i(\mathbf{k_{vac}}\cdot\mathbf{n})t} \begin{pmatrix} e^{\pi i P_0 t} & 0 & 0 & \cdots \\ 0 & e^{\pi i P_g t} & 0 & \cdots \\ 0 & 0 & e^{\pi i P_h t} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} C_0^{(1)} & C_0^{(2)} & C_0^{(3)} & \cdots \\ C_g^{(1)} & C_g^{(2)} & C_g^{(3)} & \cdots \\ C_h^{(1)} & C_h^{(2)} & C_h^{(3)} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\times \begin{pmatrix} e^{2\pi i \lambda^{(1)} t} & 0 & 0 & \cdots \\ 0 & e^{2\pi i \lambda^{(2)} t} & 0 & \cdots \\ 0 & 0 & e^{2\pi i \lambda^{(3)} t} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix} \begin{pmatrix} \alpha^{(1)} \\ \alpha^{(2)} \\ \alpha^{(3)} \\ \vdots \end{pmatrix}$$

α: weighting coefficients
t: Specimen thickness