Basic concept of HRTEM simulation

Common parameters/functions

λ Wave length of incident electron

C_s Spherical aberration coefficient

C_c Chromatic aberration coefficient

β Illumination semi-angle due to the finite source size effect

ΔE $1/e$ width of electron energy fluctuations

Δ_0 $1/e$ width of defocus spread assuming Gaussian distribution

$$\Delta_0 = C_c \frac{\Delta E}{E}$$

Δf Defocus value

Δf_{sch} Scherzer focus :

$$\Delta f_{sch} = -2\sqrt{C_s \lambda / 3}$$

$\mathbf{R}$ Vector on XY plane in real space

$\mathbf{K}$ Vector projected to XY plane of incident wave vector

$\mathbf{G}, \mathbf{H}$ Vector projected to XY plane of reciprocal lattice vectors

$\chi(\mathbf{u})$ Lens aberration function:

$$\chi(\mathbf{u}) = \pi\lambda\Delta f u^2 + \frac{1}{2}\pi\lambda^3 C_s u^4 = \pi\lambda u^2(\Delta f + \lambda^2 C_s u^2/2)$$

$A(\mathbf{u})$ Aperture function :

$$A(\mathbf{u}) = \begin{cases} 1 & (\mathbf{u} \text{ is inside obj. aperture}) \\ 0 & (\mathbf{u} \text{ is outside obj. aperture}) \end{cases}$$

T_g Transmission coefficient (see also next page) :

$$T_g(z = t; \mathbf{k}) = \sum_j \alpha^{(j)}(\mathbf{k}) C_g^{(j)}(\mathbf{k}) \exp\left[2\pi i\left(k_z - k_{0,z} + g_z + \lambda^{(j)}(\mathbf{k})\right)t\right]$$

Quasi-coherent model

$I(\mathbf{R})$ Intensity of HRTEM image :

$$I(\mathbf{R}) = |\psi(\mathbf{R})|^2$$

$\psi(\mathbf{R})$ Incident electron wavefunction on image plane :

$$\psi(\mathbf{R}) = \sum_g T_g \exp[2\pi i(\mathbf{K}+\mathbf{G})\cdot\mathbf{R}]\ \exp[-i\chi(\mathbf{K}+\mathbf{G})]\ A(\mathbf{K}+\mathbf{G})\ E_c(\mathbf{K}+\mathbf{G})\ E_s(\mathbf{K}+\mathbf{G})$$

$E_c(\mathbf{u})$: Coherence function for temporal coherence :

$$E_c(\mathbf{u}) = \exp[-(\pi\lambda\Delta_0 u^2)^2/2],$$

$E_s(\mathbf{u})$: Coherence function for spatial coherence :

$$E_s(\mathbf{u}) = \exp[-\pi^2\beta^2 u^2(\Delta f + \lambda^2 C_s u^2)^2]$$

Transmission cross coefficient model

$I(\mathbf{R})$ Intensity of HRTEM image :

$$I(\mathbf{R}) = \sum_g \sum_h T_g T_h^* \exp[2\pi i(\mathbf{G}-\mathbf{H})\cdot\mathbf{R}]\, TCC(\mathbf{K}+\mathbf{G}, \mathbf{K}+\mathbf{H})$$

$TCC(\mathbf{u}, \mathbf{u}')$ Transmission cross coefficient :

$$TCC(\mathbf{u}, \mathbf{u}') = A(\mathbf{u})A(\mathbf{u}')\exp[-i\{\chi(\mathbf{u}) - \chi(\mathbf{u}')\}]\, E_c^M(\mathbf{u}, \mathbf{u}') E_s^M(\mathbf{u}, \mathbf{u}')$$

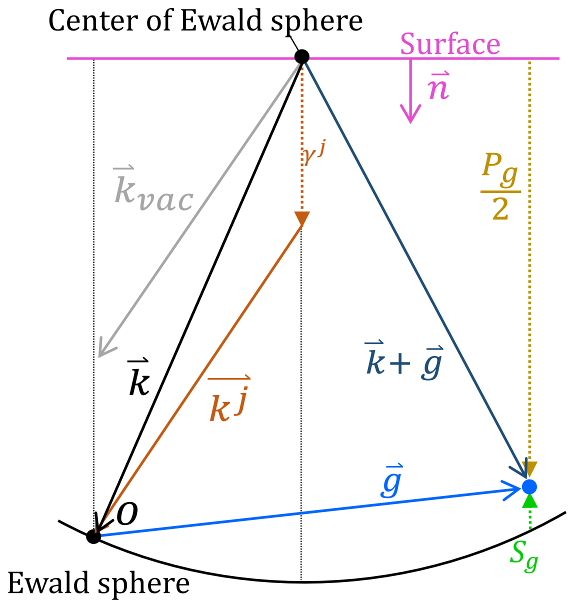
$E_c^M(\mathbf{u}, \mathbf{u}')$ Mixed coherence function for temporal coherence :

$$E_c^M(\mathbf{u}, \mathbf{u}') = \exp\left[-(\pi\lambda\Delta_0)^2\left(u^2 - u'^2\right)^2/2\right]$$

$E_s^M(\mathbf{u}, \mathbf{u}')$ Mixed coherence function for spatial coherence :

$$E_s^M(\mathbf{u}, \mathbf{u}') = \exp[-\pi^2\beta^2\{\Delta f(\mathbf{u}-\mathbf{u}') + \lambda^2 C_s(u^2\mathbf{u} - u'^2\mathbf{u}')\}^2]$$

Definitions of vectors and scalars



$\longrightarrow$ Vector

$\cdots\rightarrow$ 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)

Eigen values/vectors equation

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

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

U_g: Crystal potential
$P,\ Q$: Defined in above figure
$\lambda^{(j)}$: j^{th} eigen value
$C_*^{(j)}$: j^{th} eigen vectors

Matrix representation of transmission coefficient T_g

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

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

k_{vac_z}: $\vec{n} \cdot \vec{k}_{vac}$
α: weighting coefficients
t: Specimen thickness

Simplification of transmission cross coefficient model

Consider diffraction beams g_n which satisfy $A(\mathbf{K}+\mathbf{G}_n)=1$

$$\mathrm{F}(\mathrm{g}_n,\mathrm{g}_m)=T_{g_n}T^*_{g_m}\exp[2\pi i(\mathbf{G}_n-\mathbf{G}_m)\cdot\mathbf{R}]\exp[-i\{\chi(\mathbf{K}+\mathbf{G}_n)-\chi(\mathbf{K}+\mathbf{G}_m)\}]$$
$$\times E_c^M(\mathbf{K}+\mathbf{G}_n,\mathbf{K}+\mathbf{G}_m)E_s^M(\mathbf{K}+\mathbf{G}_n,\mathbf{K}+\mathbf{G}_m)$$

- $T_{g_n}T^*_{g_n}=\left|T_{g_n}\right|^2$
- $\exp[2\pi i(\mathbf{G}_n-\mathbf{G}_n)\cdot\mathbf{R}]=1$
- $\exp[-i\{\chi(\mathbf{u})-\chi(\mathbf{u})\}]=1$
- $E_s^M(\mathbf{u},\mathbf{u})=1$
- $E_c^M(\mathbf{u},\mathbf{u})=1$

➔ $\mathrm{F}(\mathrm{g}_n,\mathrm{g}_n)=\left|T_{g_n}\right|^2$

- $T_gT_h^*=\left(T_hT_g^*\right)^*$
- $\exp[2\pi i(\mathbf{G}_n-\mathbf{G}_m)\cdot\mathbf{R}]=\{\exp[2\pi i(\mathbf{G}_n-\mathbf{G}_m)\cdot\mathbf{R}]\}^*$
- $\exp[-i\{\chi(\mathbf{u})-\chi(\mathbf{u}')\}]=\{\exp[-i\{\chi(\mathbf{u}')-\chi(\mathbf{u})\}]\}^*$
- $E_c^M(\mathbf{u},\mathbf{u}')=E_c(\mathbf{u}',\mathbf{u})$
- $E_s^M(\mathbf{u},\mathbf{u}')=E_s(\mathbf{u}',\mathbf{u})$

➔ $\mathrm{F}(\mathrm{g}_n,\mathrm{g}_m)+\mathrm{F}(\mathrm{g}_m,\mathrm{g}_n)$

$$=\mathrm{F}(\mathrm{g}_n,\mathrm{g}_m)+\{\mathrm{F}(\mathrm{g}_m,\mathrm{g}_n)\}^*=2\times\Re\big(\mathrm{F}(\mathrm{g}_m,\mathrm{g}_n)\big)$$

where $\Re(a+b\,i)=a$

Therefore, a computation load of the TCC model can be reduced as follows;

$$I(\mathbf{R})=\sum_{n=1}^{N}\sum_{m=1}^{N}T_{g_n}T^*_{g_m}\exp[2\pi i(\mathbf{G}_n-\mathbf{G}_m)\cdot\mathbf{R}]\,TCC(\mathbf{K}+\mathbf{G}_n,\mathbf{K}+\mathbf{G}_m)$$

$$=\sum_{n=1}^{N}\left|T_{g_n}\right|^2+2\sum_{n=1}^{N}\sum_{m=n+1}^{N}\Re\left\{T_{g_n}T^*_{g_m}\exp[2\pi i(\mathbf{G}_n-\mathbf{G}_m)\cdot\mathbf{R}]\,TCC(\mathbf{K}+\mathbf{G}_n,\mathbf{K}+\mathbf{G}_m)\right\}$$

Furthermore, same value of $\exp[2\pi i(\mathbf{G}_n-\mathbf{G}_m)\cdot\mathbf{R}]$ are repeated many times in the above summation. By storing the value, the calculation speed can be further accelerated.