Advanced Analysis in TEM

05/22/2020

Week 5

(S)TEM image Simulations
Part III

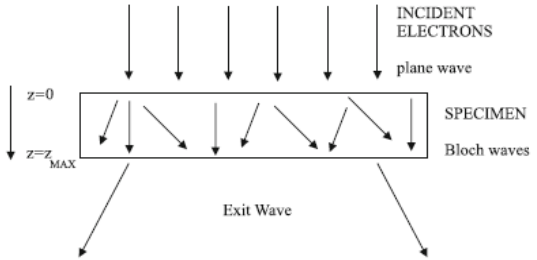
(S)TEM Simulation of Thick Specimens
Implementation of Multislice method (concepts)

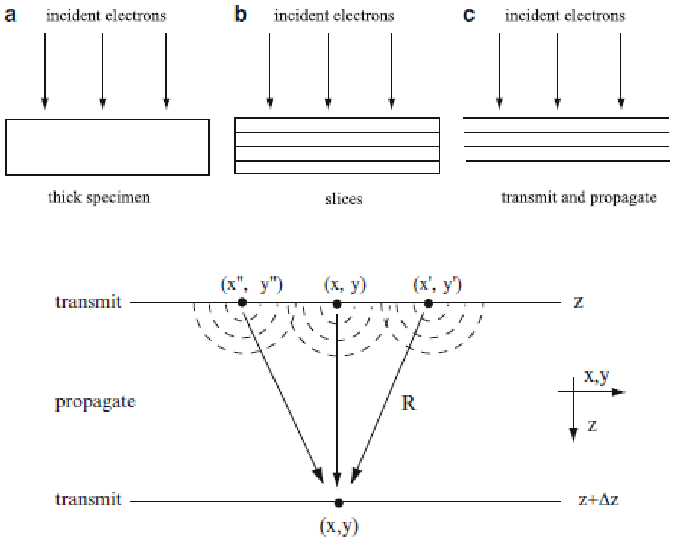
Theory of Calculation of Thick Images

e^- interacts strongly with the specimen and can scatter more than once as it passes through specimens (dynamical)

Multislice

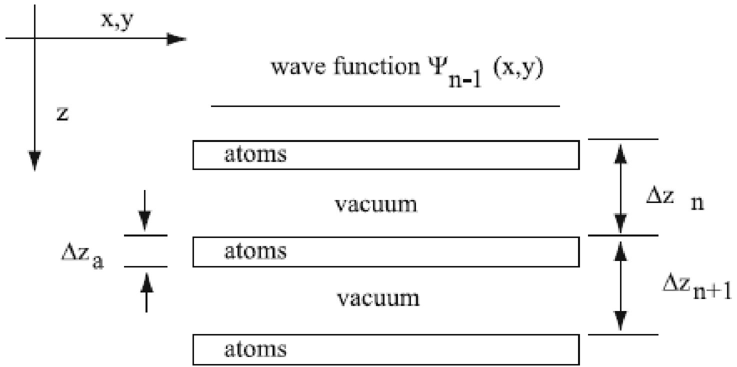
Bloch Wave

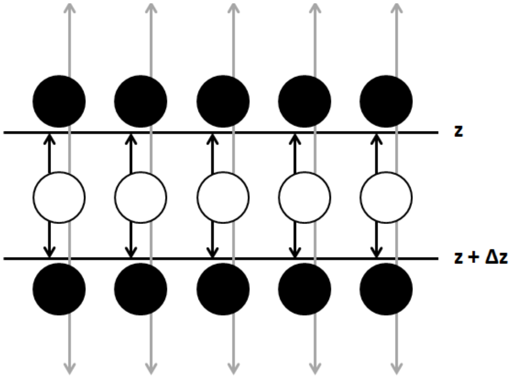




Multislice Method: Steps

Slicing the Specimen





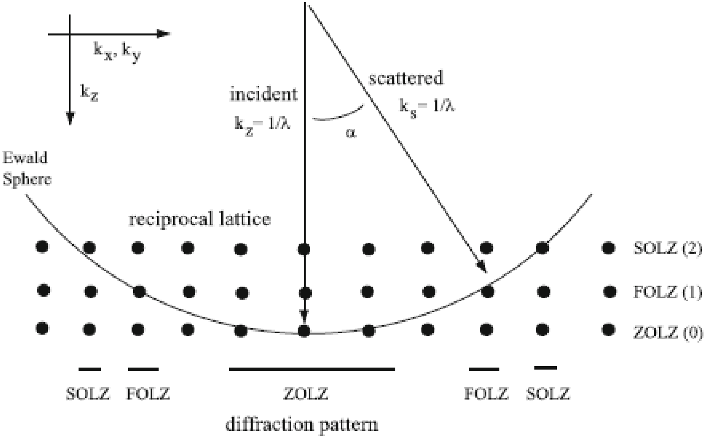
Multislice Method: Steps

Probing HOLZ

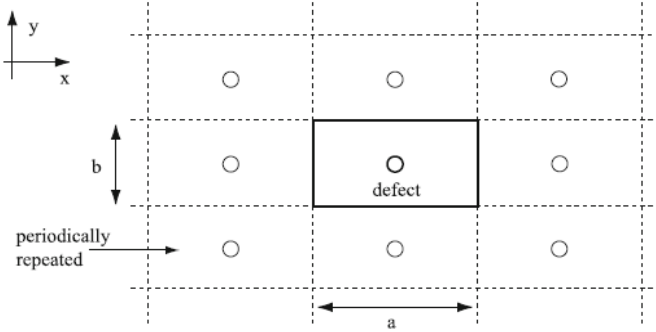
HOLZ will be reproduced if slice thickness matches the natural sample periodicity

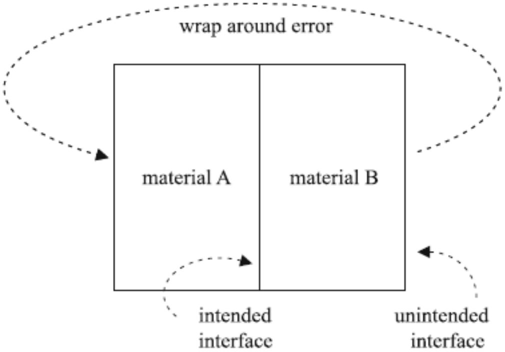
Projected potential

$$v_{\Delta z}(x,y) = \int_{z}^{z+\Delta z} V(x,y,z)\mathrm{d}z \sim \int_{-\infty}^{+\infty} V(x,y,z)\mathrm{d}z = v_z(x,y).$$



Interfaces and Defects





Multislice Implementation

Step 1	Divide the specimen into thin slices.
Step 2	Calculate the projected atomic potential $v_{zn}(\mathbf{x})$ [(5.19) or (5.21)] for each slice and symmetrically bandwidth limit them.
Step 3	Calculate the transmission function $t_n(\mathbf{x}) = \exp[i\sigma v_{zn}(\mathbf{x})]$ (5.25) for each slice and symmetrically bandwidth limit each to 2/3 of it maximum to prevent aliasing.
Step 4	Initialize the incident wave function $\psi_0(x,y) = 1$.
Step 5	Recursively transmit and propagate the wave function through each slice $\psi_{n+1}(x,y) = p_n(x,y,\Delta z_n) \otimes [t_n(x,y)\psi_n(x,y)]$ using FFT's as in (6.92). Repeat until the wave function is all the way through the specimen
Step 6	Fourier transform the wave function at the exit surface of the specimen $\Psi_n(k_x,k_y) = \mathrm{FT}[\psi_n(x,y)]$.
Step 7	Multiply the transmitted wave function $\Psi_n(k_x,k_y)$ by the transfer function of the objective lens, $H_0(k)$ (5.27) to get the image wave function in the back focal plane $\Psi_i(\mathbf{k}) = H_0(k)\Psi_n(\mathbf{k})$.
Step 8	Inverse Fourier transform the image wave function $\psi_i(\mathbf{x}) = \mathrm{FT}^{-1}[\Psi_i(\mathbf{k})]$.
Step 9	Calculate the square modulus of the image wave function (in real space) to get the final image intensity $g(\mathbf{x}) = \lvert\psi_i(\mathbf{x})\rvert^2 = \lvert\psi_n(\mathbf{x}) \otimes h_o(\mathbf{x})\rvert^2$.

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