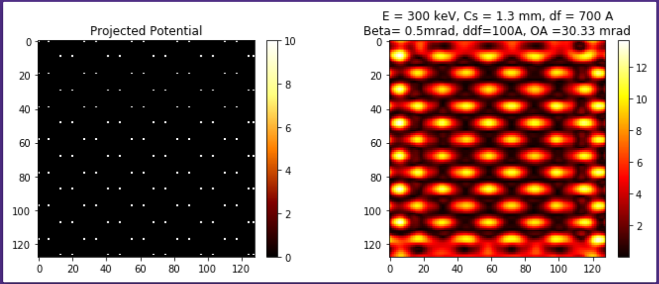
Advanced Analysis in TEM

05/15/2020



SHyNE Soft and Hybrid Nanotechnology Experimental Resource
NUANCE Atomic and Nanoscale Characterization Experimental Center

Northwestern McCORMICK SCHOOL OF ENGINEERING

Week 4

(S)TEM image Simulations

Part II

TEM Simulation of Thin Specimens

Calculation of Images of Thin Specimens

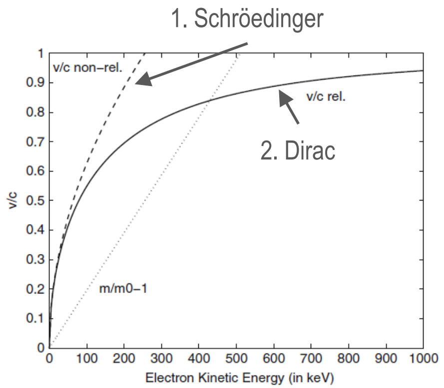
General Conditions:

- Neglects geometrical thickness of the specimen (i.e. **very thin**)
- Ignores **multiple scattering**, intermediate approach between the transfer function and the *multislice* and *Bloch wave* methods

Outcomes:
- **Qualitative** insight into the structure in the image and it requires much less computer time!
- Calculation of the transmission function of thin specimens is also a **necessary** part of more advanced calculations

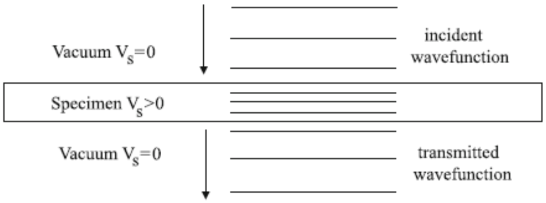
Calculation of Images of Thin Specimens

Kinect Energy of imaging electrons



1. Accurate enough in the typical energy ranges used in the electron microscope
2. Significantly more difficult to work with mathematically

e⁻ primary interaction: electrostatic potential of the specimen and the charge on the electron.



$$\psi(\mathbf{x}) \sim \exp(2\pi i k_z z)\exp(i\sigma V_s z), \quad \text{where} \quad \sigma = \frac{2\pi}{\lambda V}\left(\frac{m_0c^2+eV}{2m_0c^2+eV}\right) = \frac{2\pi m e\lambda}{h^2}$$

For a very thin specimen:

$$\psi_t(\mathbf{x}) = t(\mathbf{x})\exp(2\pi i k_z z)$$
$$t(\mathbf{x}) = \exp[i\sigma v_z(\mathbf{x})]$$

Projected Atomic Potential:

Integral along the optic axis, z of the specimen:

$$v_z(\mathbf{x}) = v_z(x,y) = \int V_s(x,y,z)\mathrm{d}z$$

In a whole image simulation:

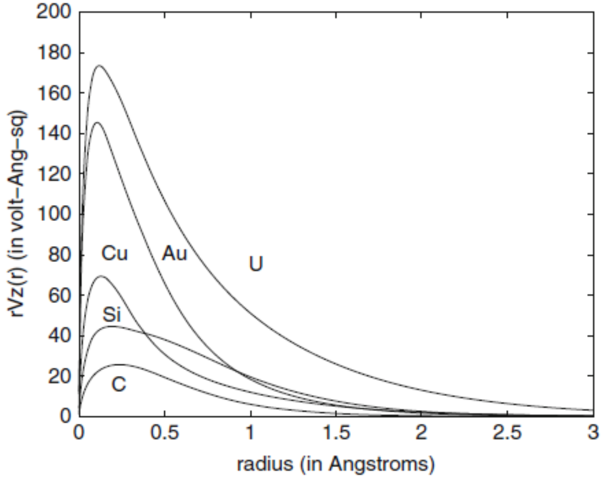
$$v_z(\mathbf{x}) = \sum_{j=1}^{N} v_{zj}(\mathbf{x}-\mathbf{x}_j)$$

Linear superposition of each atom in the specimen

WARNING

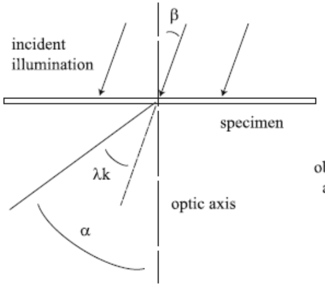
5-10% error in image quantification in the low scattering (e.g CTEM, STEM-BF)

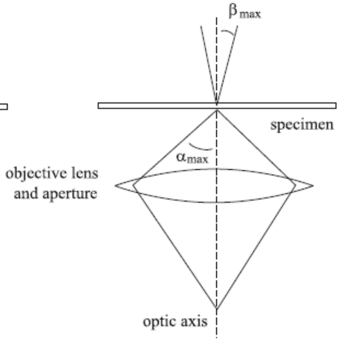
Relative contribution to an image.



Coherent vs Incoherent Illumination

Incident electrons are not perfectly parallel!





Transmission wave function:

$$\psi_t(\mathbf{x}) = t(\mathbf{x})\psi_{\text{inc}}(\mathbf{x}) \rightarrow \psi_t(\mathbf{x}) = t(\mathbf{x})\exp(2\pi i \mathbf{k}_\beta \cdot \mathbf{x}).$$

Lateral Coherence

$$\Delta x_{\text{coh}} \sim \frac{0.16\lambda}{\beta_{\max}}.$$

$$\beta_{\max} \ll 0.16\alpha_{\max} \quad \text{coherent imaging}$$
$$\beta_{\max} \gg 0.16\alpha_{\max} \quad \text{incoherent imaging}$$

α_{max} is the maximum objective angle (OA)

ΔE == to a small (incoherent) Δd

β_{max}/α_{max} controls coherence

Born M, Wolf E (1980) Principles of optics, 6th ed. Pergamon Press, Oxford

It's Coding Time!