

Introduction to image simulation: why image simulation?

Winter School on High Resolution Electron Microscopy

Held at the

John M. Cowley Center for High Resolution Electron Microscopy

January 5 - 10, 2020

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December 20, 2019

Image simulation in High Resolution Electron Microscopy:

- 1 **Helps understand** experimental images (diffraction or micrograph).
- 2 **Provides valuable information** about several crystal parameters pretty difficult to assess by any other technique (precise **crystal orientation**, **crystal thickness**, **atomic columns** position, atomic species, etc).
- 3 **Is particularly useful** when dealing with crystal defects (dislocations, interfaces or particles).

Image simulation is often necessary, particularly when using aberrations corrected microscopes.

To perform HRTEM image simulation it is necessary to acquire a deep understanding of:

- 1 **Crystallography** (how to create crystal models).
- 2 **Electron diffraction** (under mainly **elastic and low angle** scattering approximations).
- 3 **Ray or geometric optics and its aberrations** (impact of optical aberrations).
- 4 **Fourier optics** (transfer of information, image formation and acquisition).

There are too many recommended good books and publications to list them all.

HRTEM image simulation: a few recommended books & publications

- J.M. Cowley, *Diffraction Physics*.
- M. De Graef, *Introduction to Conventional Transmission Electron Microscopy*.
- P.B. Hirsch, A. Howie, R.B. Nicholson, W.D. Pashley & M.I. Whelan, *Electron Microscopy of Thin Crystals*.
- E.J. Kirkland, *Advanced Computing in Electron Microscopy*.
- J.-P. Morniroli, *Large-Angle Convergent-Beam Electron Diffraction*.
- S.J. Pennycook & P.D. Nellist, *Scanning Transmission Electron Microscopy*.
- J.C.H. Spence, *High Resolution Electron Microscopy*.
- J.M. Zuo, J.C.H. Spence, *Advanced Transmission Electron Microscopy*.
- Z.L. Wang, *Elastic and Inelastic Electron Scattering in Electron Diffraction and Imaging*.

Books on crystallography that you may find useful:

- D.E. Sands, *Introduction to Crystallography*, Dover Books on Chemistry.
- D.E. Sands, *Vectors and Tensors in Crystallography*, Dover Publications Inc.

Recommended publications:

- J.M. Cowley & A.F. Moodie, *Acta Cryst.* **10**, (1957) 609-619.
- D. Gratias & R. Portier, *Acta Cryst.* **A39** (1983) 576-584.
- K. Ishizuka, *Ultramicroscopy* **5** (1980) 55-65, *Ultramicroscopy* **90** (2002) 71-83.
- D. Van Dyck, *Phys. Status Solidi* **72** (1975) 321-336.
- P.G. Self, M.A. O'Keefe, P.R. Buseck, A.E.C. Spargo, *Ultramicroscopy* **11** (1983) 35-52.

Ideally, HRTEM characterisation should follow steps (1) \rightarrow (5):

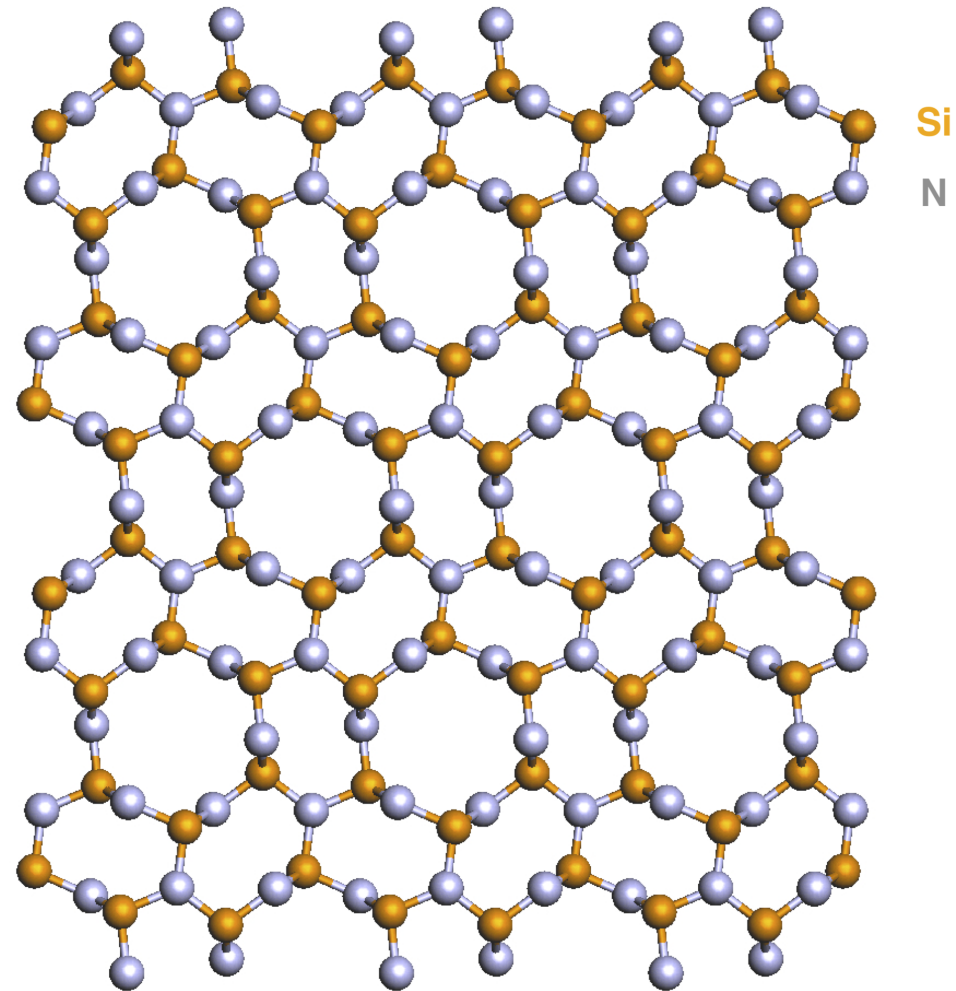
- 1 Image(s) acquisition (one or a defocus series).
- 2 Wave-function(s) recovery.
- 3 Projected potential (inverse scattering?).
- 4 Atoms (x, y, z coordinates) & atomic number.
- 5 Comparison with a model.

Unfortunately instrumental settings, aberrations, instabilities, multiple scattering, etc, make the ideal path (1) \implies (4) difficult or (even) hazardous to follow.

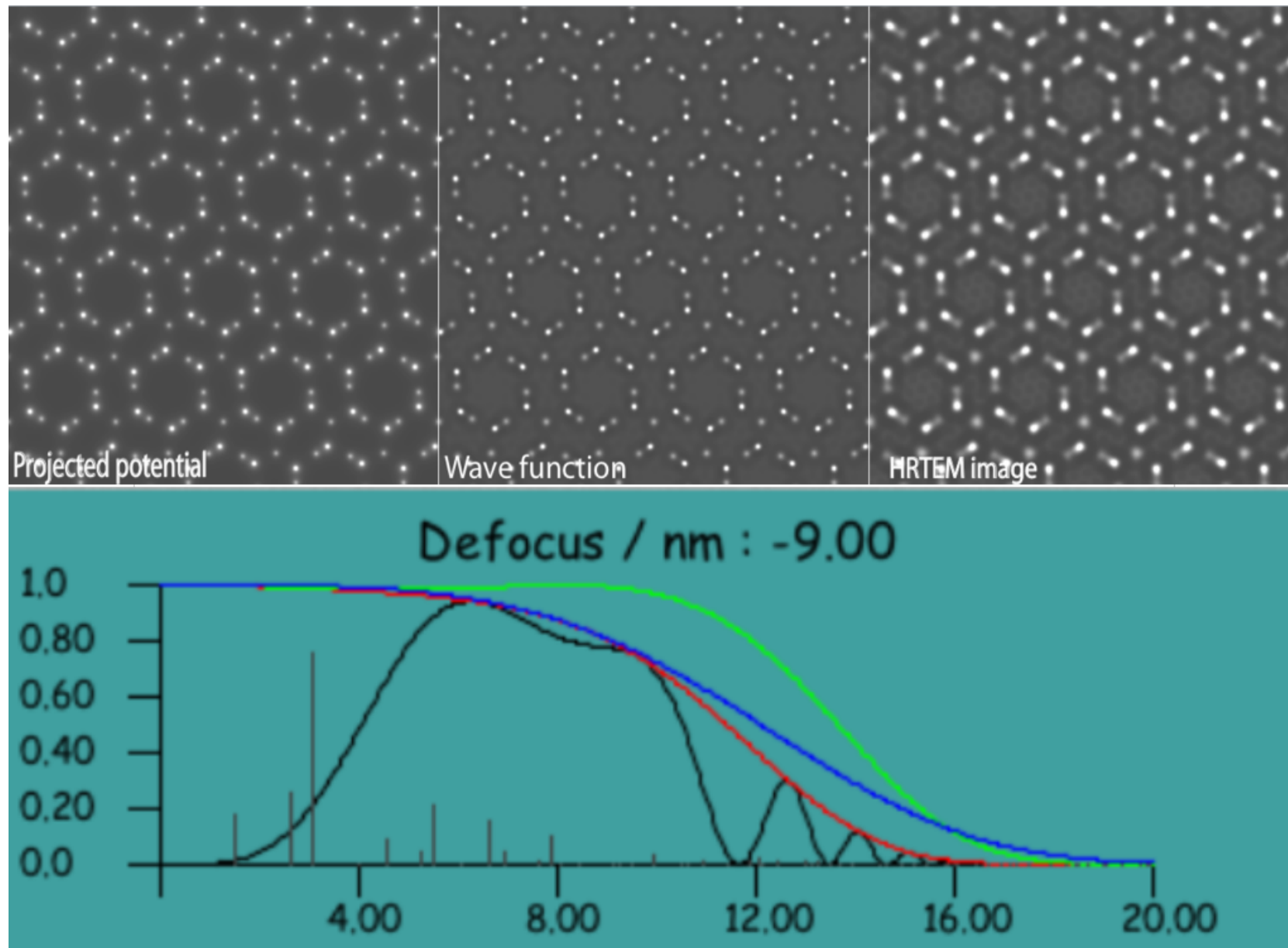
HRTEM image simulation follows the **reverse (& easier!) path (5) \implies (1).**

Example: Si_3N_4 P 63: [001], effect of 6 nm defocus

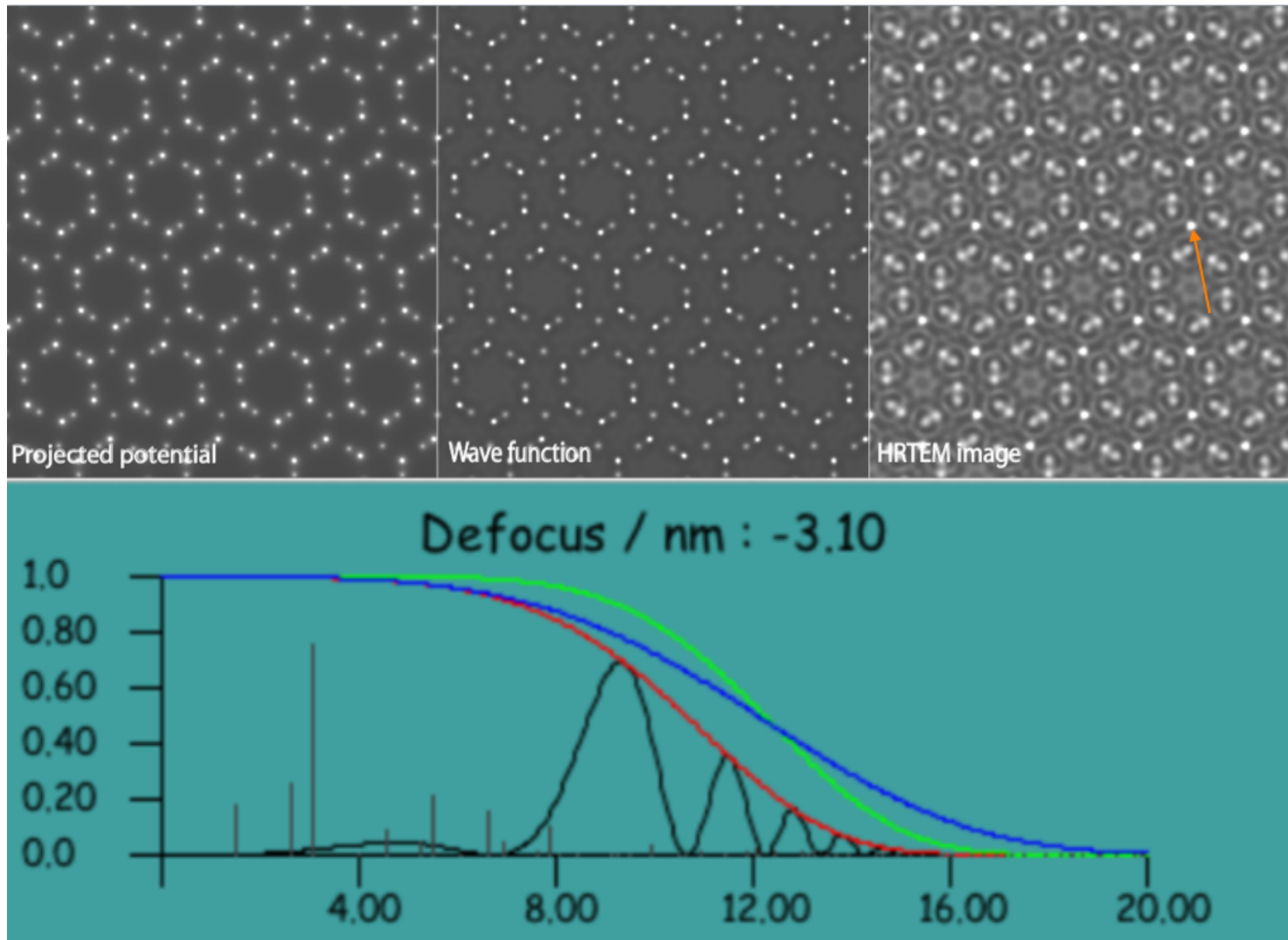
HR(S)TEM images depend of several adjustable microscope parameters and images **DO NOT** always show faithfully the crystal structure.



Small changes of imaging conditions (defocus 6 nm) strongly affects HRTEM imaging.



Imaging parameters: Titan 80-300 (300 kV), C_s : $-33 \mu\text{m}$. The transfer function plot (modulus) shows the imaging conditions and the spatial frequencies that are properly transferred.



Imaging parameters: Titan 80-300 (300 kV), C_s : $-33 \mu\text{m}$. Note that the contrast of the **nitrogen** atoms is now higher than the Si contrast (**arrow**).

HR(S)TEM image simulation: a necessity?

We will consider 3 structures and show that image simulation helps understand HRTEM images.

Remember we observe images, we can under favorable circumstances recover the wave-function that results of the interaction of the incident (plane) electron wave with the **crystal potential**.

The 3 structures are very simple but **hexagonal**.

In hexagonal crystals (hkl) plane normals are not parallel to [uvw] directions where (h=u, k=v & l=w) (except (001) // [001]).

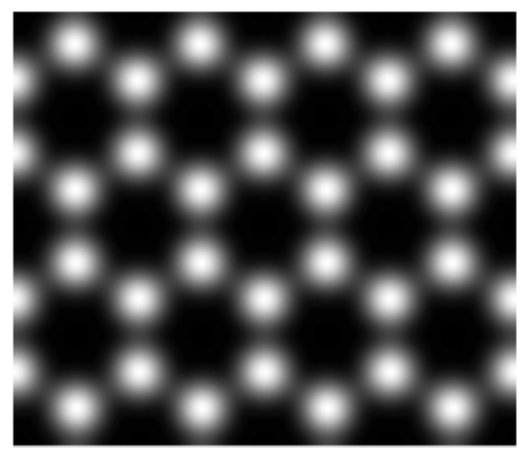
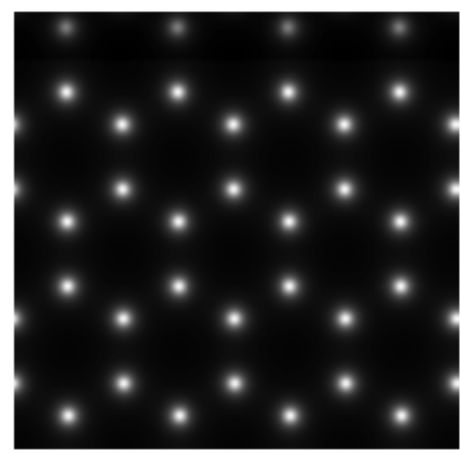
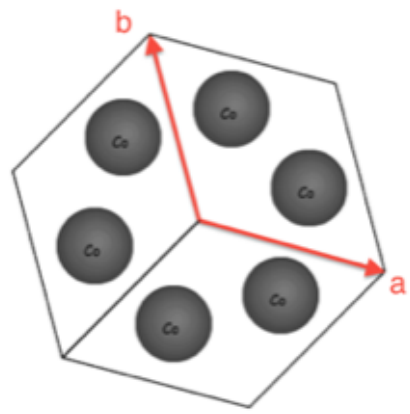
- **Simple structure: Co [001] & [120]**
- **Slightly more complicated structure: $MgZn_2$ [001] & [120]**
- **Structure ? & [uvw] ?**

When simple structures are imaged, image simulation may not be necessary at all.

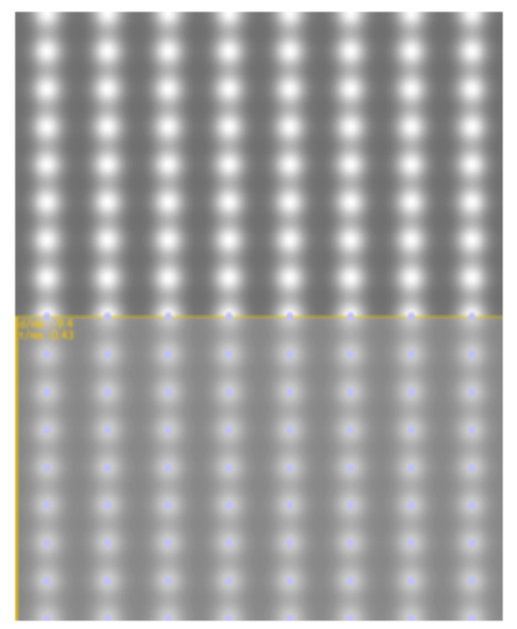
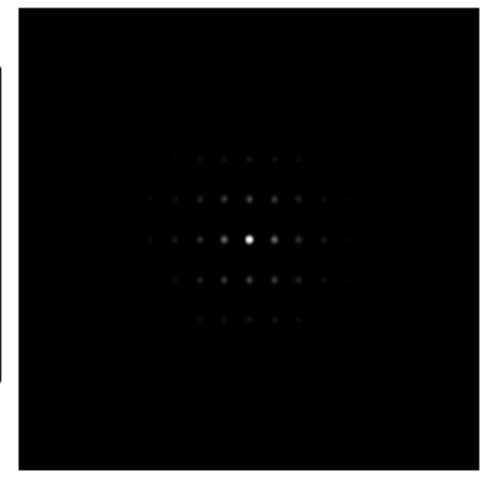
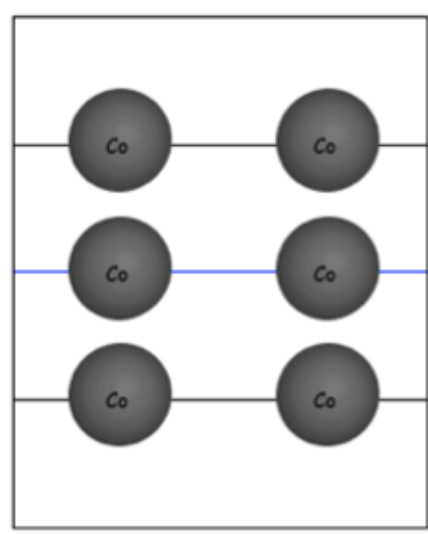
For example looking at Co (P63/mmc, magnetic!), model structure, projected potential, SAED, HRTEM are simple (and straight forward to interpret).

Under optimum imaging conditions the position of the atomic columns is directly accessible.

Simple structure: Co [001] & [120] or Weber [10-10]



Co [001]



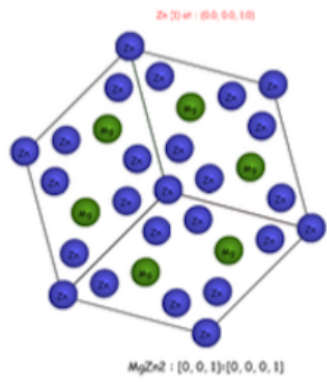
Co [120]

Projected potential

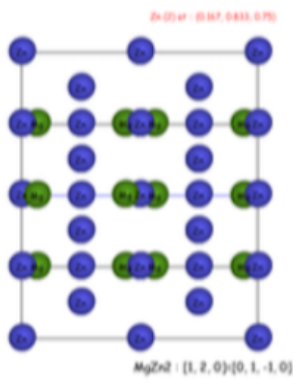
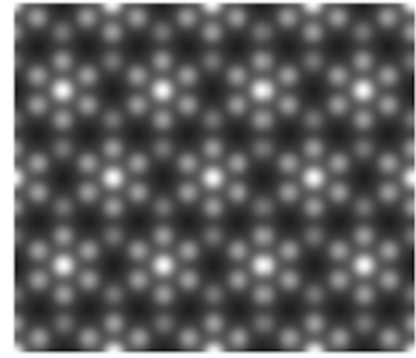
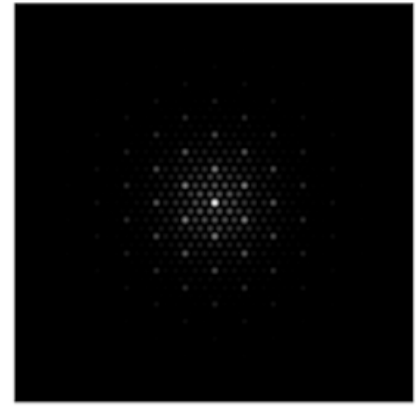
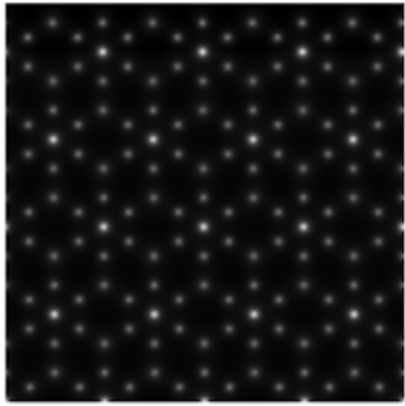
SAED

HRTEM

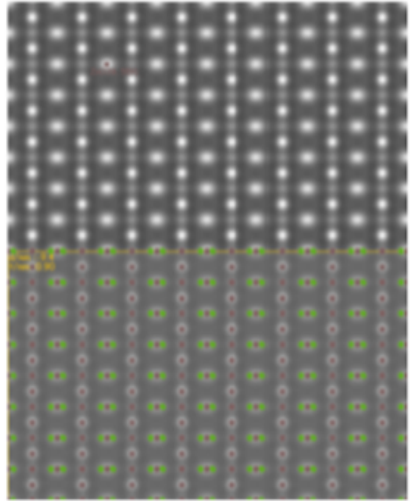
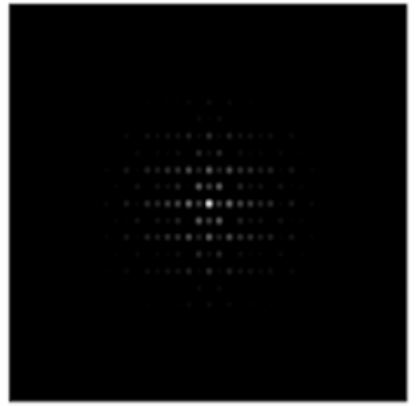
(A little) more complicated structure: $MgZn_2$ [001] & [120]



$MgZn_2$ [001]



$MgZn_2$ [120]

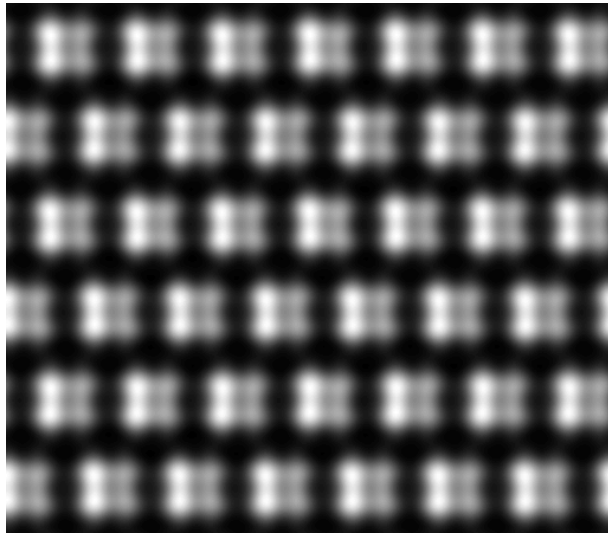


Projected potential

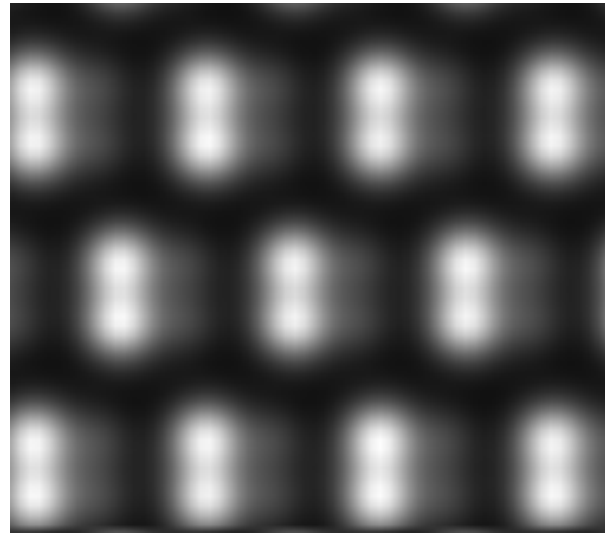
SAED

HRTEM

What is the structure giving these HRTEM & HRSTEM images?



HRTEM (negative Cs).



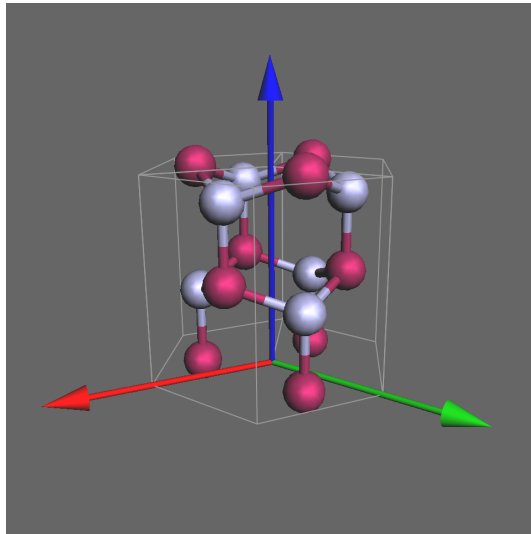
STEM: annular dark field.



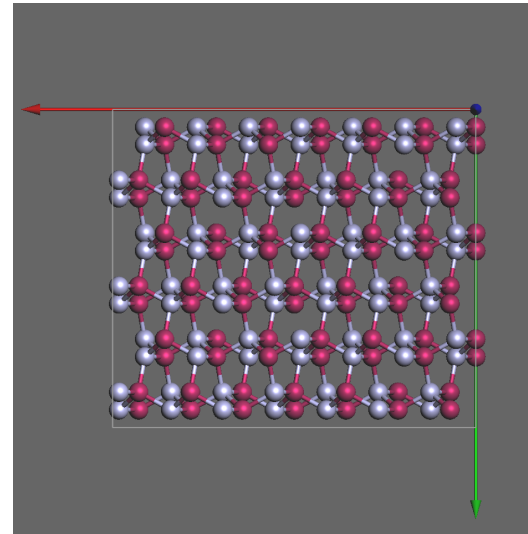
STEM: bright field.

Crystal $[uvw]$ orientation and atomic columns' type & position?

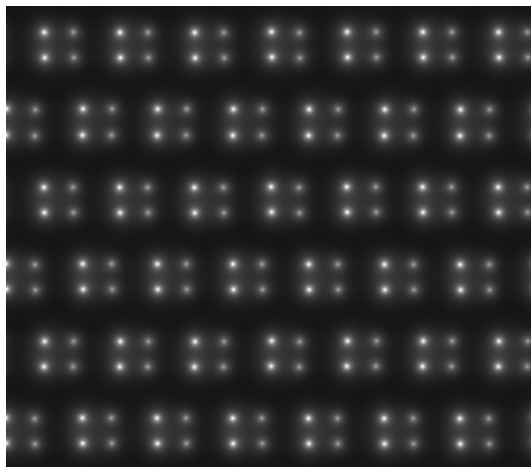
AlN: Important opto-electronics structure



AlN: $P6_3mc$



AlN: $[1,1,1] = [1, 1, -2, 3]$.



AlN: projected potential.



AlN: SAED diffraction pattern.

Experimental images K. Urban (Juelich group)

How to do HRTEM, HRSTEM or HAADF image simulation?

We need models, (good) approximations and methods.

1 Models

• Crystal:

- Lattice parameters.
- Symmetries (space-group, regular point system).
- Atoms position.
- Orientation, ([uvw] zone axis indices, (hkl) Laue circle center indices with $u h + v k + w l = 0$).
- Shape (thickness, defect, ...).

• Microscope:

- Accelerating voltage.
- Source coherence (i.e. source size, energy spread).
- Illumination convergence.
- Objective lens properties (C_s (W_{40}): spherical aberration coefficient, C_c (W_{00}): chromatic aberration coefficient, ...).

• Detector: Modulation Transfer Function (MTF).

2 Diffraction & imaging: approximations

1 Elastic scattering (small angle scattering, i.e. acc. voltage ≥ 50 kV):

- Kinematical: single scattering event.
- Dynamical: multiple scattering events.

2 Inelastic scattering (frozen lattice or frozen phonon approximations):

- Single inelastic scattering event.
- Multiple inelastic scattering events.

3 Abbe imaging theory (transmission cross-coefficients or transfer function + envelopes).

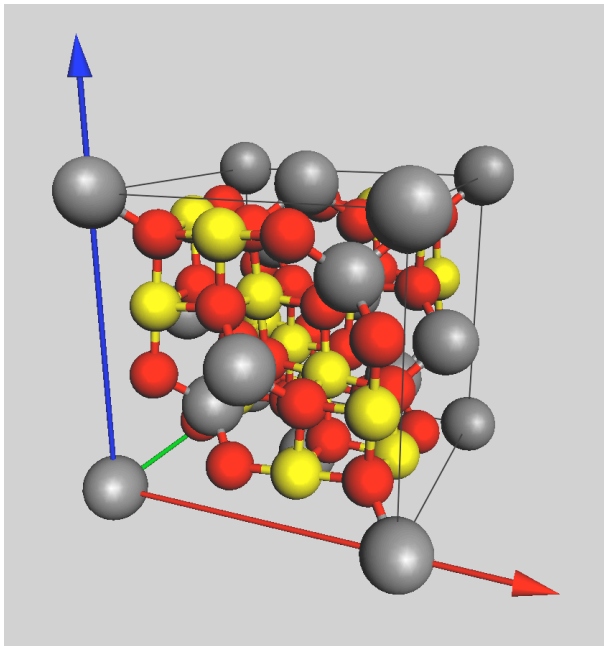
3 Most popular methods

- 1 Bloch-wave (solid state physics).
- 2 Multislice (physical optics).

- ① → **Atomic model.**
- ② Scattering and dynamical diffraction.
- ③ Image formation.
- ④ Image acquisition.

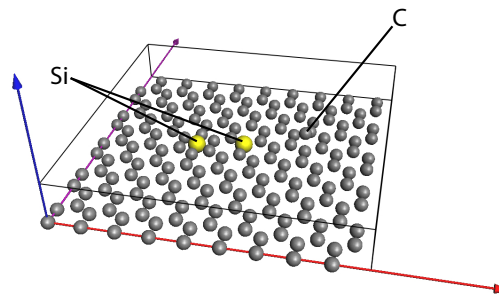
Atomic model: Crystal or atoms in a box?

Models are **not** necessarily crystalline. But they are assumed to be **periodic** (periodic continuation)!



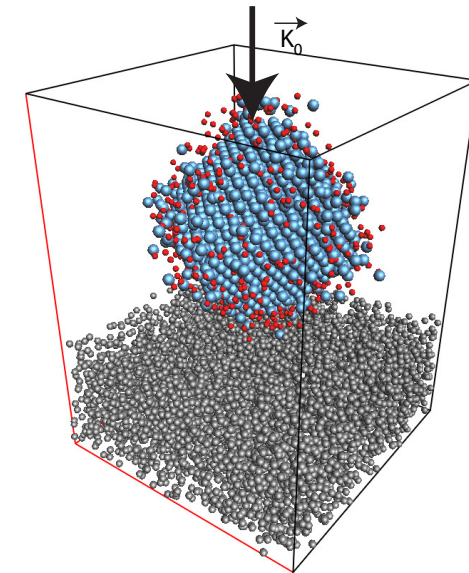
Single unit-cell

CoCr_2O_4 (cubic, Fd-3m, 3 atoms).



Simple super-cell

graphene sheet with add atoms (448 atoms).



Large super-cell

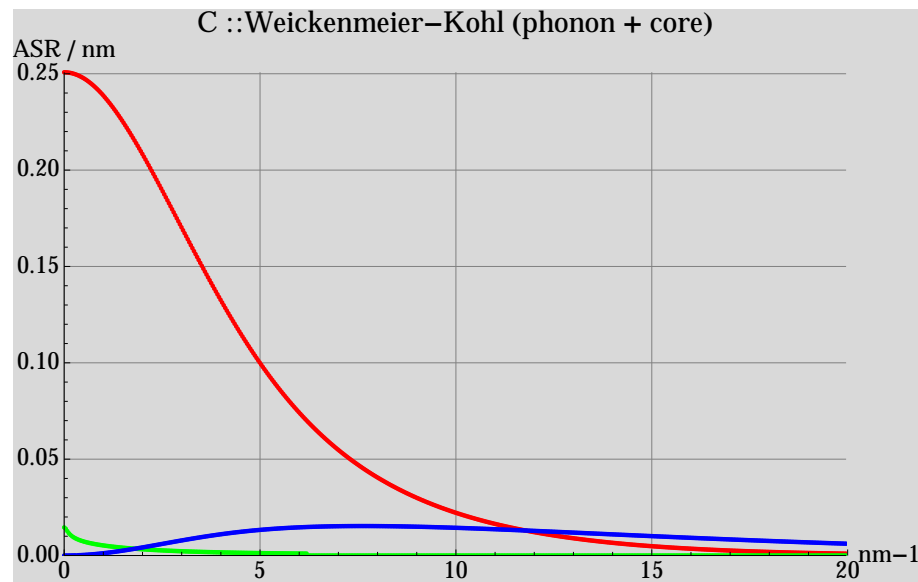
Pt catalyst (Pt cube octahedron on amorphous carbon film, $\approx 10'000$ atoms).

A model is a **box** of parameters ($a, b, c, \alpha, \beta, \gamma$) with atoms at (x, y, z) such that $0.0 \leq (x, y, z) < 1.0$. Knowing the symmetries (space-group) helps define the structure, the extinctions, etc. Wrong models **do not** provide reliable HRTEM or HRSTEM simulated images!

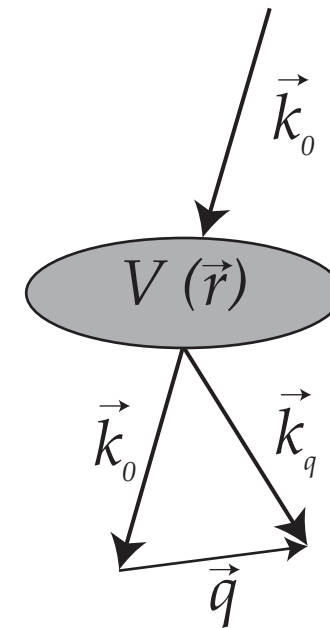
- ① Atomic model.
- ② → **Scattering and dynamical diffraction.**
- ③ Image formation.
- ④ Image acquisition.

Scattering: Atomic Scattering Amplitude

The first step of any image calculation consists in computing the scattering potential of the crystal $V(\vec{r})$. This is done within the **First Born approximation** that allows to calculate the crystal potential provided the **Atomic Scattering Amplitude** (or **Atomic Scattering Factors**) of the atoms are known. Tabulations of the ASA have been published by many authors, a good one is given by **A.L. Weickenmeier and H. Kohl**, Acta Cryst. **A47** (1991) 590-597.



Atomic Scattering Amplitude (carbon),
red: elastic, green: core absorption,
blue: TDS (Thermal Diffuse Scattering).



Electrons interact with
the crystal potential
 $V(\vec{r})$.

Scattering: $\vec{k}_q = \vec{k}_o + \vec{q}$

Elastic scattering: $|\vec{k}_q| = |\vec{k}_o|$

Schrödinger equation & Born series & first Born approximation

Time independent Schrödinger equation (time independent flux of incident electrons with no energy dispersion):

$$-\frac{\hbar^2}{2m}\vec{\nabla}^2\psi(\vec{r}) + \hat{V}(\vec{r})\psi(\vec{r}) = E\psi(\vec{r}) \quad (1)$$

The general solution can be expressed in term of a **Green's function**:

$$\psi(\vec{r}) = \phi_{inc}(\vec{r}) + \frac{2m}{\hbar^2} \int G(\vec{r} - \vec{r}') V(\vec{r}') \psi(\vec{r}') d^3r' \quad (2)$$

with $\phi_{inc}(\vec{r}) = e^{i\vec{k}_0 \cdot \vec{r}}$. The total scattered wave is finally expressed as:

$$\psi(\vec{r}) = \phi_{inc}(\vec{r}) - \frac{m}{2\pi\hbar^2} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \psi(\vec{r}') d^3r' \quad (3)$$

The equation 3 is solved approximately by a series of iterative approximations (**Born series**):

- **zero order**: $\psi_0(\vec{r}) = \phi_{inc}(\vec{r})$
- **first order**: $\psi_1(\vec{r}) = \phi_{inc}(\vec{r}) - \frac{m}{2\pi\hbar^2} \int \frac{e^{ik|\vec{r}-\vec{r}'|}}{|\vec{r}-\vec{r}'|} V(\vec{r}') \phi_{inc}(\vec{r}') d^3r'$

First Born approximation & atomic scattering amplitude

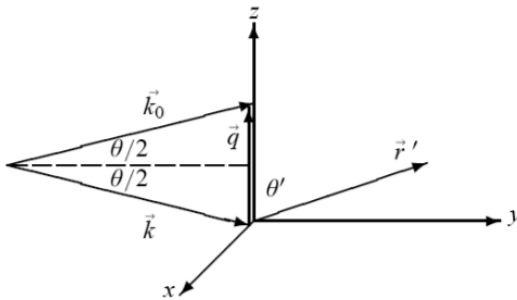
When \vec{r} is much larger than \vec{r}' i.e. ($k|\vec{r} - \vec{r}'| \approx kr - \vec{k} \cdot \vec{r}'$) and ($\frac{1}{|\vec{r} - \vec{r}'|} \approx \frac{1}{r}$) the **First Born approximation** gives the asymptotic limit of the wave function:

$$\psi(\vec{r}) = \phi_{inc}(\vec{r}) - \frac{m}{2\pi\hbar^2} \frac{e^{ikr}}{r} \int e^{-i\vec{k} \cdot \vec{r}'} V(\vec{r}') \phi_{inc}(\vec{r}') d^3r' \quad (4)$$

$$\psi(\vec{r}) = \frac{e^{i\vec{k}_0 \cdot \vec{r}}}{r} + \frac{e^{ikr}}{r} f(\theta, \phi) \quad (5)$$

$$f(\theta, \phi) = -\frac{m}{2\pi\hbar^2} \int e^{-i\vec{k} \cdot \vec{r}'} V(\vec{r}') \phi_{inc}(\vec{r}') d^3r' \quad (6)$$

The momentum transfer q for elastic scattering ($k_0 = k$) is $q = |\vec{k}_0 - \vec{k}| = 2k \sin(\frac{\theta}{2})$
 If the potential $V(\vec{r})$ is **spherically symmetric** and **weak**, i.e. $V(\vec{r}) = V(r)$ and $|V| \ll \frac{\hbar^2 k^2}{2me}$ the potential of one atom is given by the inverse Fourier transform of the atomic scattering amplitude.



$$f(g) \approx \int e^{-i\vec{g} \cdot \vec{r}} V(r) d^3r \rightarrow V(r) \approx \int e^{i\vec{g} \cdot \vec{r}} f(g) d^3g \quad (7)$$

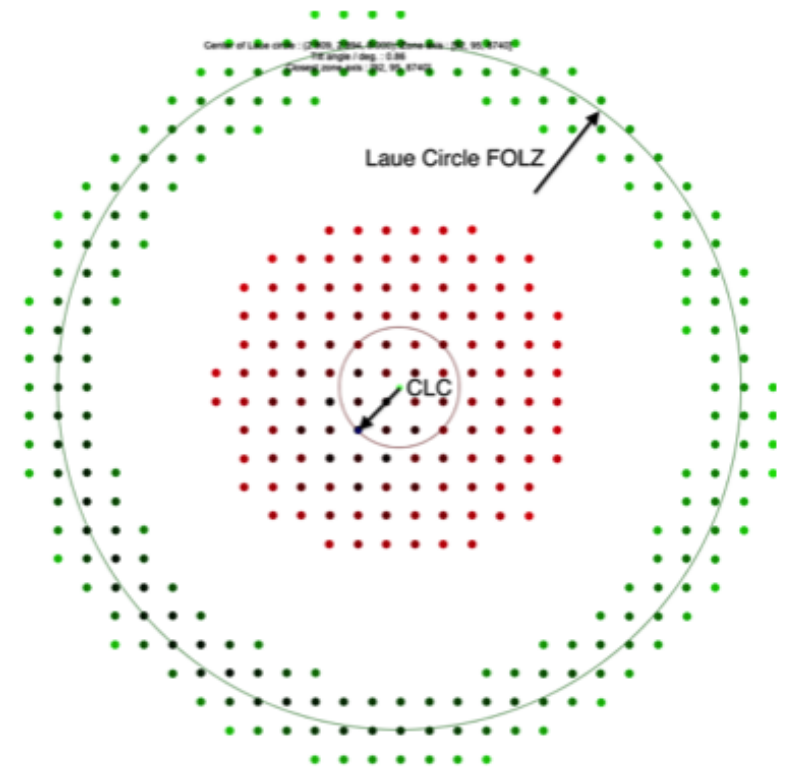
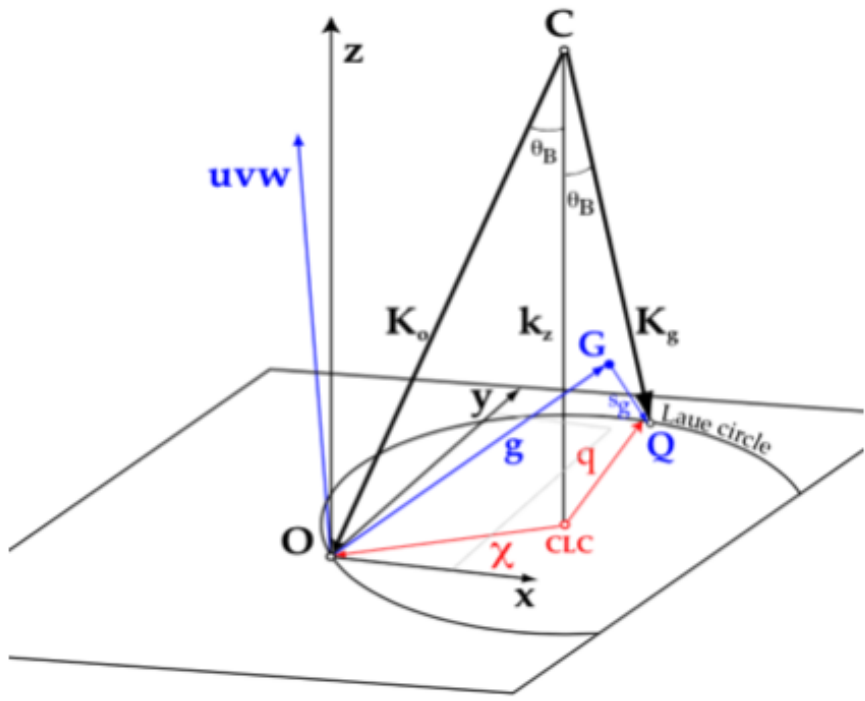
The potential of one unit cell is then calculated by adding the atomic potential of its atoms. This can be done either in Fourier space using the **structure factors** or in real space by patching the potential of the atoms at their (x,y,z) position in the unit cell.

$$F_{hkl} = \sum_{atom} f_{atom}(s) e^{-[2i\pi(hx+ky+lz)]} \quad (8)$$

with $s = \frac{\sin\theta}{\lambda}$

Diffraction geometry: zone axis $[u, v, w]$ and CLC (h, k, l)

Using the atomic form factors the crystal potential, $V_v(\vec{r})$, is generated for a particular zone axis $[u, v, w]$ and diffraction condition CLC (h, k, l).



C: center of the Ewald sphere and CLC: C projection onto the zero order Laue zone (Center of Laue Circle). Intensity $\approx |F_{hkl}(g)|^2$ single scattering approximation

Dynamical diffraction: small angle scattering

Making the small angle scattering approximation ($\psi(\vec{r}) = e^{ik_z z} \psi(\vec{\rho}, z)$ with $\vec{\rho} \perp k_z$) and neglecting backscattering ($\frac{\partial^2}{\partial z^2} \psi(\vec{\rho}, z) \approx 0$), the Schrödinger equation becomes:

$$i \frac{\partial}{\partial z} \psi(\vec{\rho}, z) = \frac{1}{2k_z} \left[-\nabla_{\rho}^2 - \chi^2 + V(\vec{\rho}, z) \right] \psi(\vec{\rho}, z) \quad (9)$$

$$i \frac{\partial}{\partial z} \psi(\vec{\rho}, z) = \hat{H}(\vec{\rho}, z) \psi(\vec{\rho}, z) \quad (10)$$

It is similar to the time dependent Schrödinger equation where coordinate z replaces time t . The causal evolution operator $\hat{U}(z, 0)$ being given by:

$$i \frac{\partial}{\partial z} \hat{U}(z, 0) = \hat{H}(\vec{\rho}, z) \hat{U}(z, 0) \quad (11)$$

When:

- $(\vec{\rho}, z)$ **does not depend** on z .
- $(\vec{\rho}, z)$ **can be neglected** (vacuum).
- $\hat{H}(\vec{\rho}, z)$ reduces to its potential term.

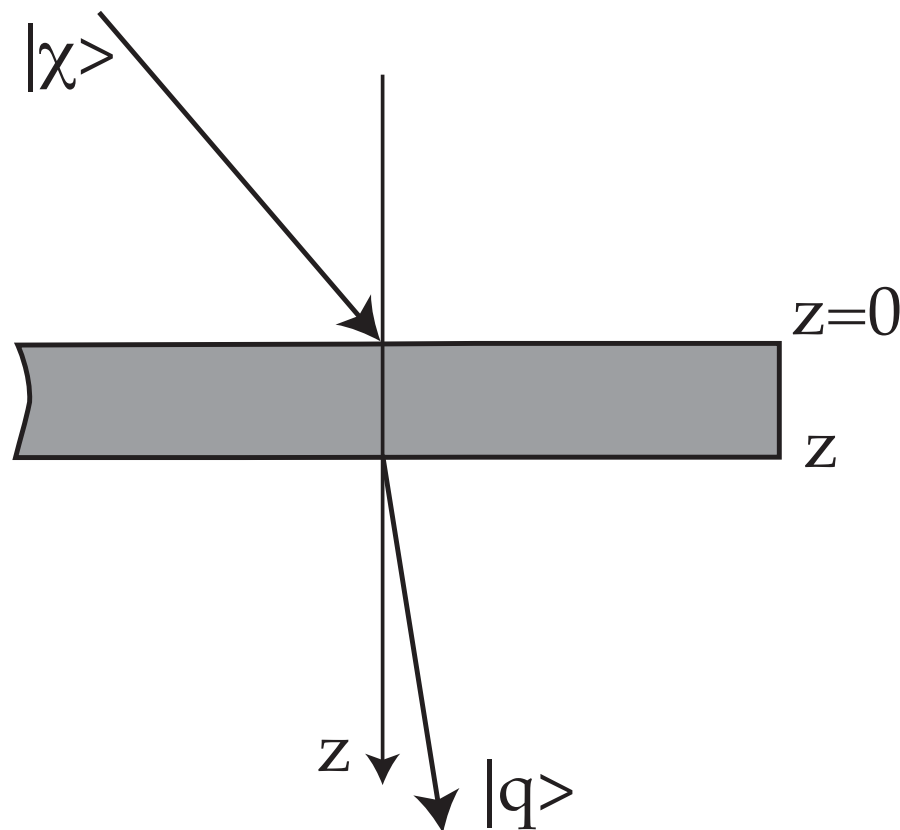
equation 11 can be integrated directly.

$$\hat{U}(z, 0) = \exp \left[-i \int_0^z \hat{H}(\vec{\rho}, \tau) d\tau \right] \quad (12)$$

Dynamical scattering: $\hat{U}(z, 0)$

The transition probability from **initial state** $|\chi\rangle$ to **final state** $|q\rangle$.

$$\omega_{\chi \rightarrow q}(z, 0) = |\langle q | \hat{U}(z, 0) | \chi \rangle|^2$$



To calculate the intensity or transition probability $\omega_{\chi \rightarrow q}(z, 0)$ we must calculate $\hat{U}(z, 0)$.

Dynamical scattering: $\langle q | \hat{U}(z, 0) | \chi \rangle$

Two popular methods to calculate $\langle q | \hat{U}(z, 0) | \chi \rangle$:

- Bloch-wave method.
- **Multislice method** (example follow).

Bloch-wave method is best suited to calculate dynamical diffraction of **small unit cell** crystals in any **[uvw]** direction. Calculation time goes as $\approx n^3$ (n number of reflections).

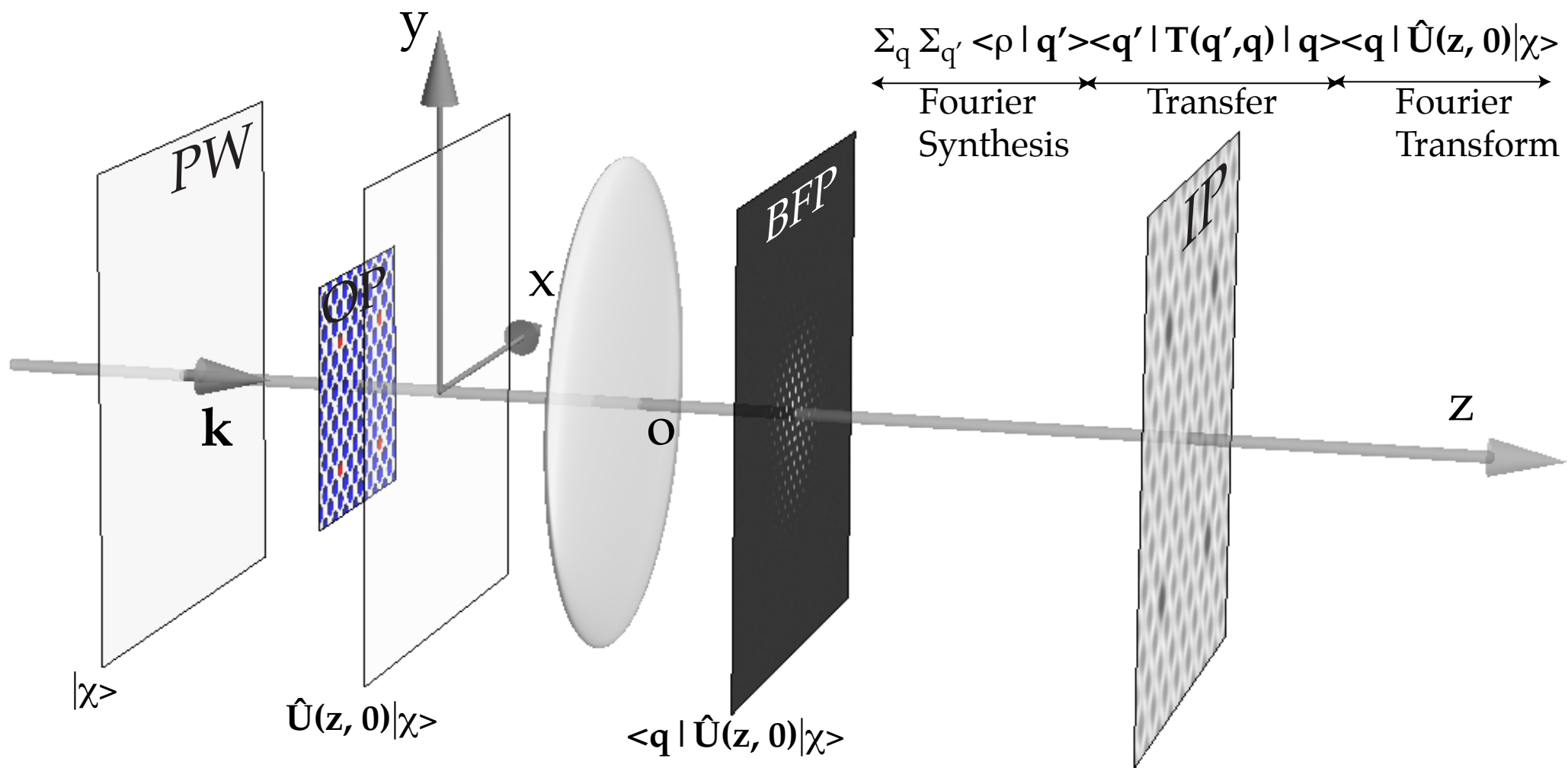
Multislice method is more efficient calculating dynamical diffraction of **crystal defects** or large unit crystals.

Dynamical diffraction including inelastic scattering gives more complicated and computer intensive calculations. See:

L.J. Allen, A.J. D'Alfonso, S.D. Findlay, *Modelling the inelastic scattering of fast electrons*, Ultramicroscopy **151** (2015) 11.

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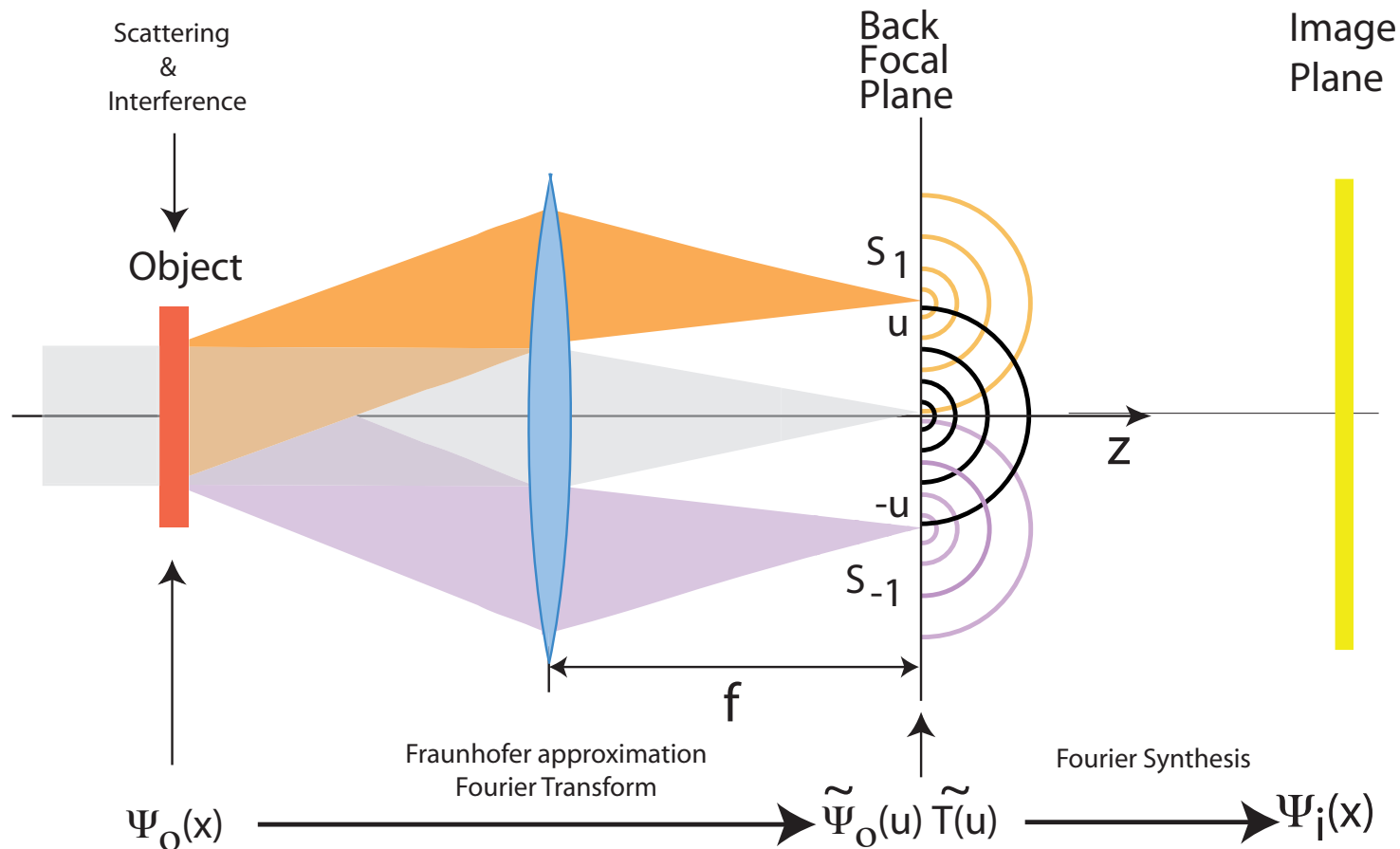
Microscope



Modelling the transfer of information by the microscope.

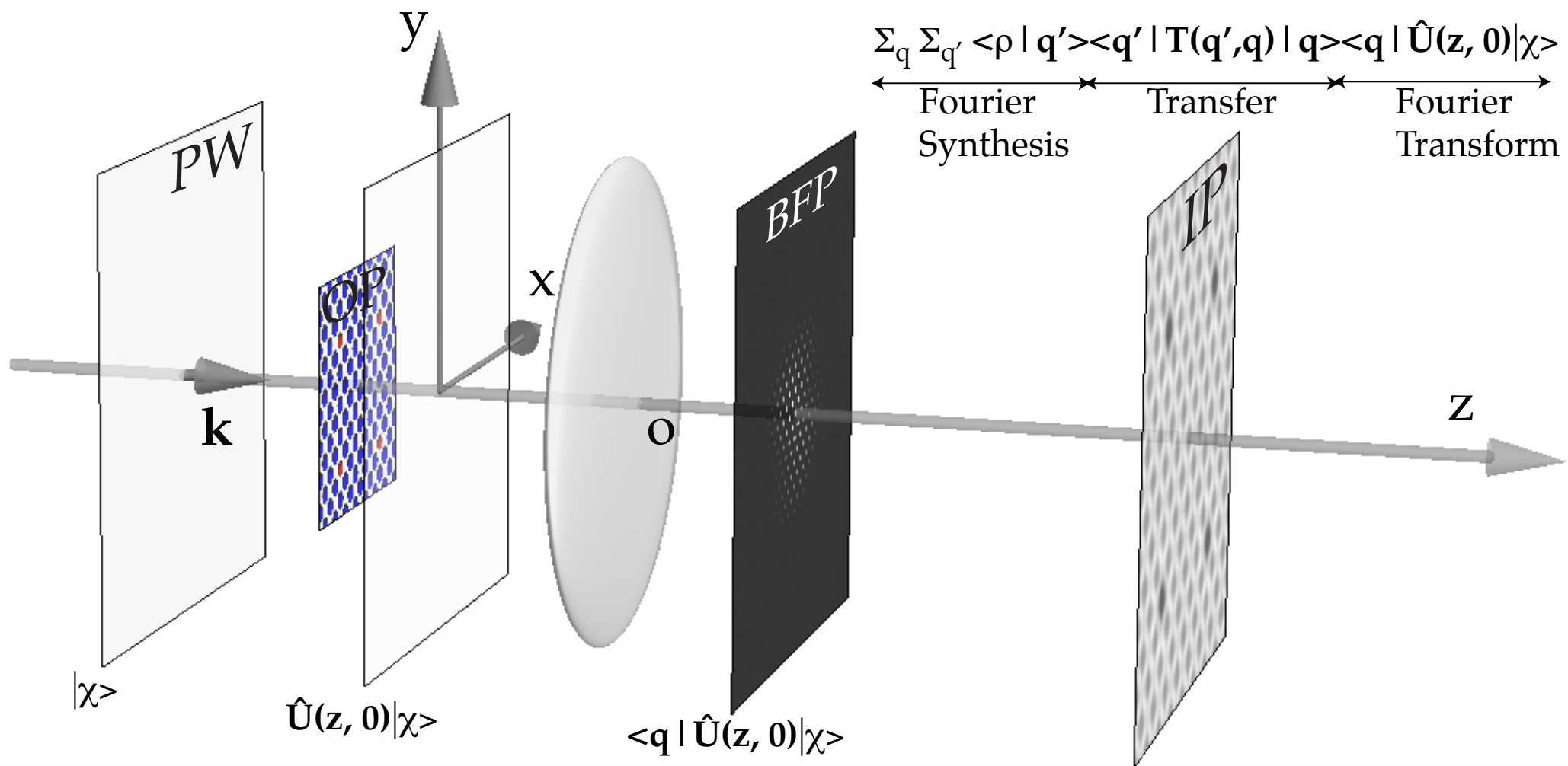
- 1 **Abbe image formation theory (≈ 1870).**
- 2 **HRTEM: transfer function** (coherent or partially coherent illumination). **Transmission cross coefficients.**
- 3 **HRSTEM: optical transfer function** (incoherent imaging process). **Partially coherent probe.**

Model: Abbe image formation



The objective lens changes the phase relationship between the transmitted and diffracted beams. Moreover not all diffracted beams are transmitted, due to its small acceptance angle. High spatial frequencies (i.e. beams diffracted at large angles) are damped due to partial spatial and temporal coherence, electronic noise, mechanical vibrations or drift.

Microscope & image formation modelling (HRTEM)



$|\chi\rangle \implies$ incident wave-function

$$|\Psi_i\rangle = \underbrace{\sum_{q'} \langle \rho | q' \rangle}_{\text{Fourier synthesis}} \underbrace{\sum_q \langle q' | \hat{T}(q', q) | q \rangle}_{\text{Objective lens transfer}} \underbrace{\langle q | \hat{U}(z, 0) | \chi \rangle}_{\text{Fourier transform}}$$

Assuming that the potential is z independent, the evolution operator $\hat{U}(z, 0)$ depends on the Hamiltonian $\hat{H}(\vec{\rho}, z)$ of the system "crystal + incident electron" (where $\vec{\rho}$ are the (x, y) coordinates in a plane perpendicular to the optical axis O_z of the microscope).

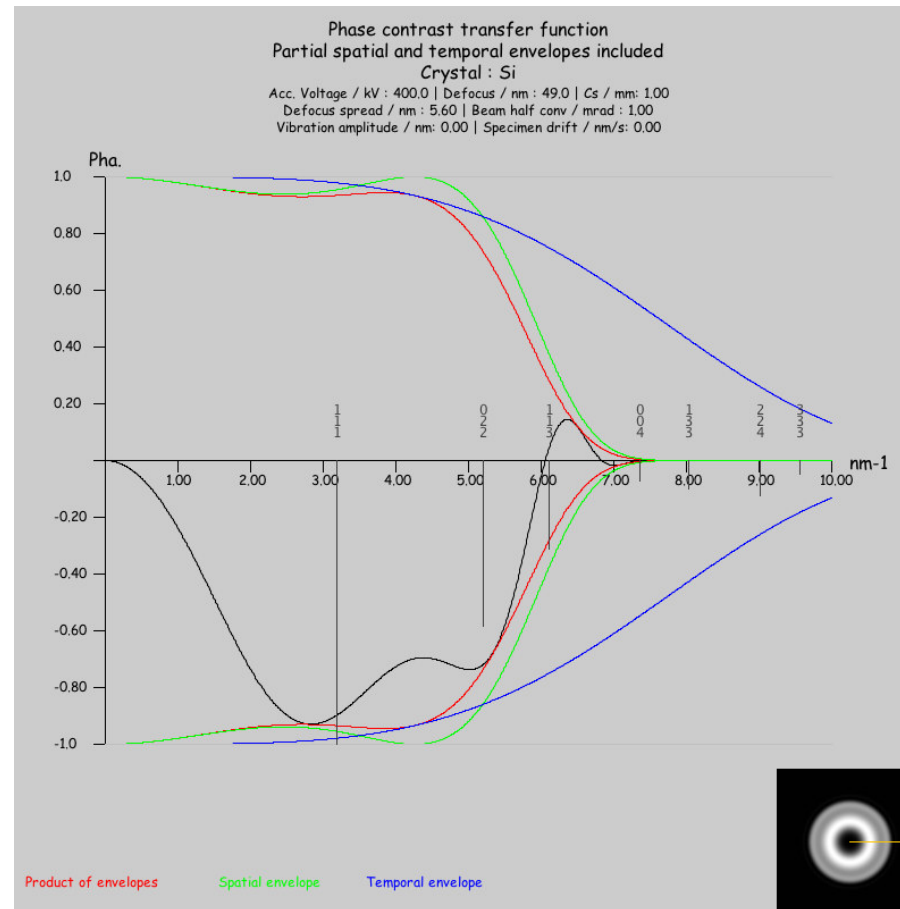
When \hat{H} does not depend on z :

$$\hat{U}(z, 0) = \exp^{-i \int_0^z \hat{H}(\vec{\rho}, z) dz} = \exp^{-i \hat{H}(\vec{\rho}) z}$$

Transfer by objective lens $T(q', q)$

The **T**ransfer **F**unction (TF) and **P**hase **C**ontrast **T**ransfer **F**unction (PCTF) are:

$$\underbrace{\sum^q \langle q' | \hat{T}(q', q) | q \rangle}_{\text{Objective lens transfer}} \implies \underbrace{\tilde{T}(\vec{u})}_{\text{TF}} = e^{-i\chi(\vec{u})} = \underbrace{\cos(\chi(\vec{u}))}_{\text{TF}} - i \underbrace{\sin(\chi(\vec{u}))}_{\text{PCTF}}$$



PCTF: $\sin(\chi(\vec{u}))$ where $\chi(\vec{u})$ collects the optical path difference of the aberrations.

Point Spread Function (PSF), image of a point source

$$(PSF(\vec{x}) = FT^{-1} [\tilde{T}(\vec{h})])$$

- Coherent illumination & attenuation envelopes:

$$\Phi_i(\vec{x}) = \Phi_o(\vec{x}) \otimes PSF(\vec{x})$$

- Partially coherent illumination T_{cc} (Transmission Cross Coefficient):

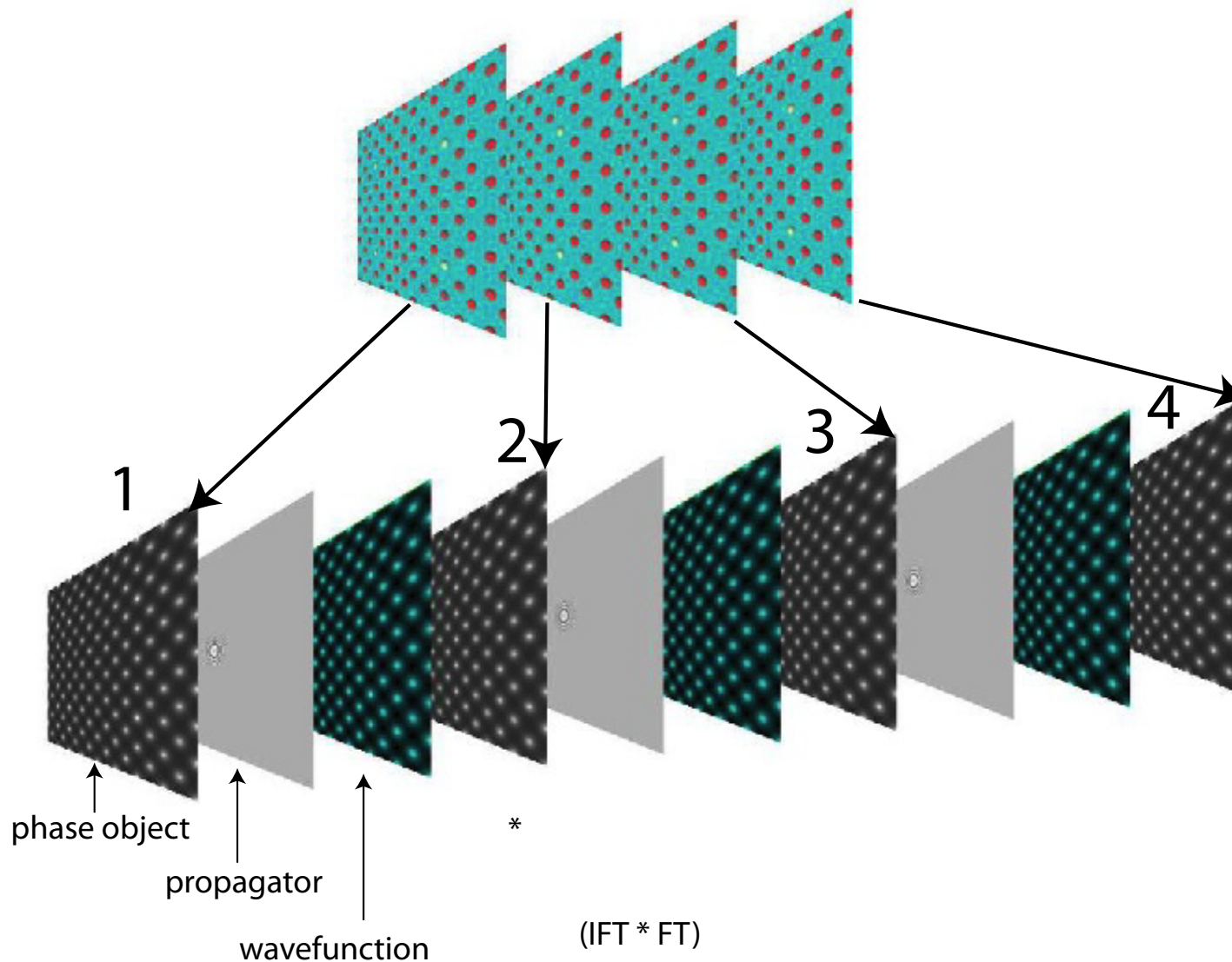
$$\tilde{I}(\vec{h}; z) = \int \tilde{T}_{cc}(\vec{h}' + \vec{h}; \vec{h}; z) \phi(\vec{h}' + \vec{h}) \phi^*(\vec{h}') d\vec{h}'$$

K. Ishizuka, Ultramicroscopy **5** (1-3), 55-65.

- Incoherent illumination (HRSTEM):

$$I(\vec{x}) = |\Phi_o(\vec{x})|^2 \otimes [PSF(\vec{x}) PSF^*(-\vec{x})]$$

Example of image simulation using the **multislice** method



A very popular (and powerful) method for performing dynamical calculations has been proposed by **J. M. Cowley** (founder of CSSS) and A.F. Moodie. It makes use of several principles of Optical Physics.

- **step 1:** define orthogonal box (periodic crystal).
- **step 2:** slice the box into thin slices ~ 0.2 nm.

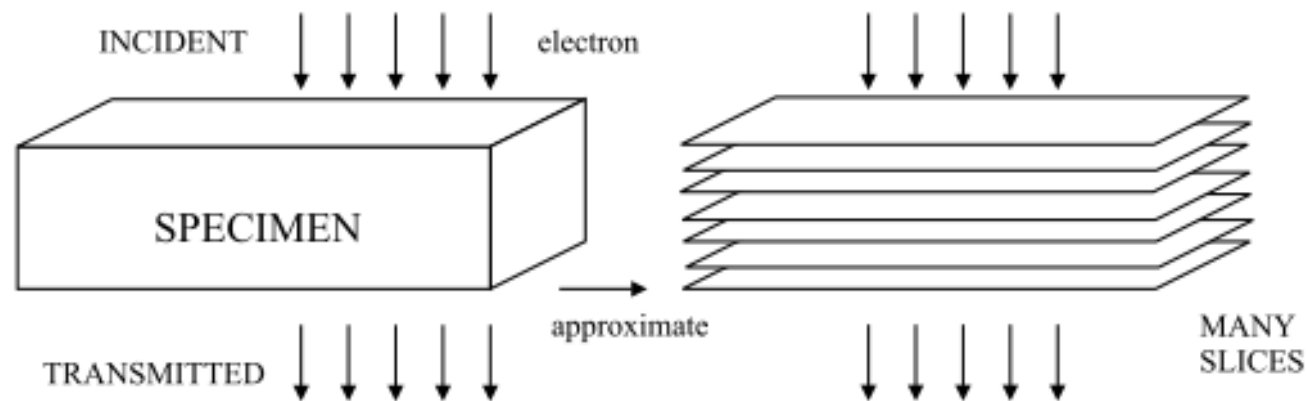


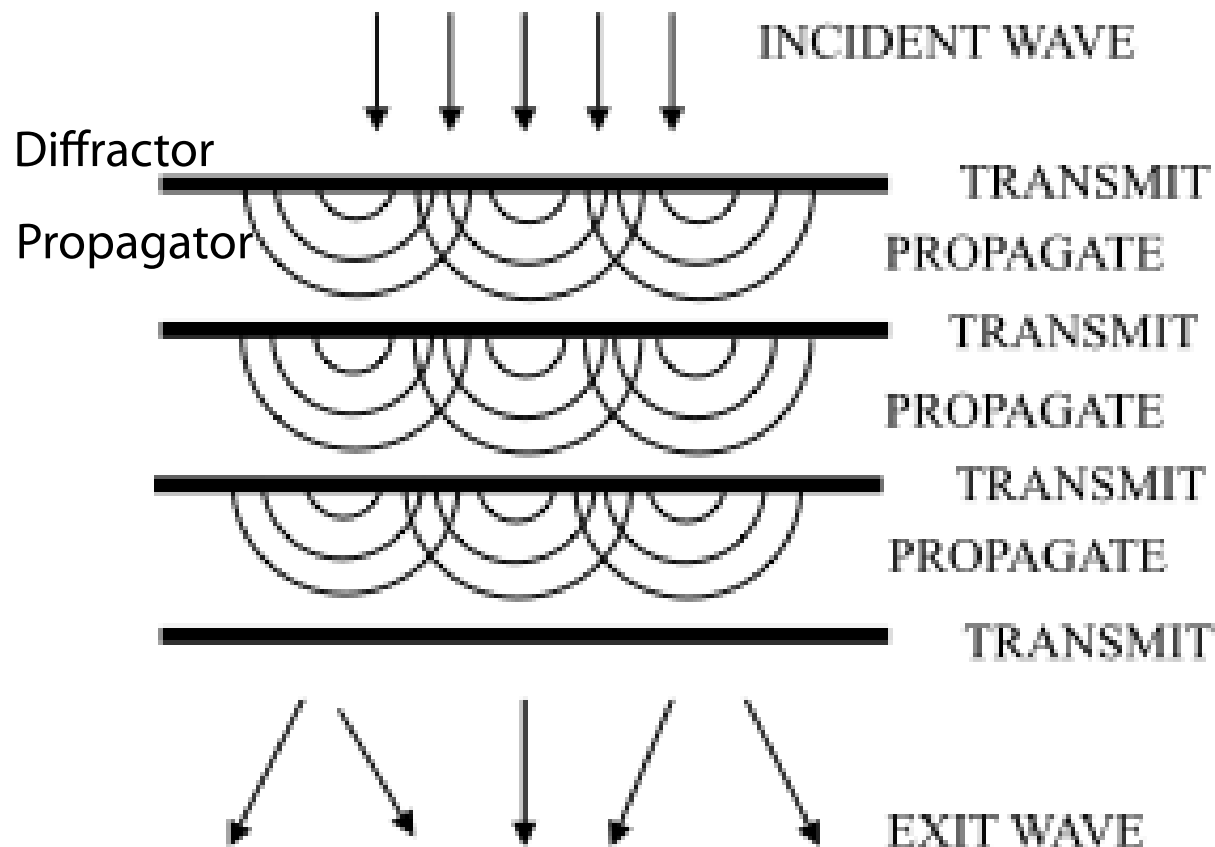
Figure: The orthogonal crystal model is sliced ¹ and the potential of the slices is projected on a plane.

¹The multislice method necessitates orthogonal & periodic crystal models in order to avoid image artefacts.

Multislice: propagating the wave function

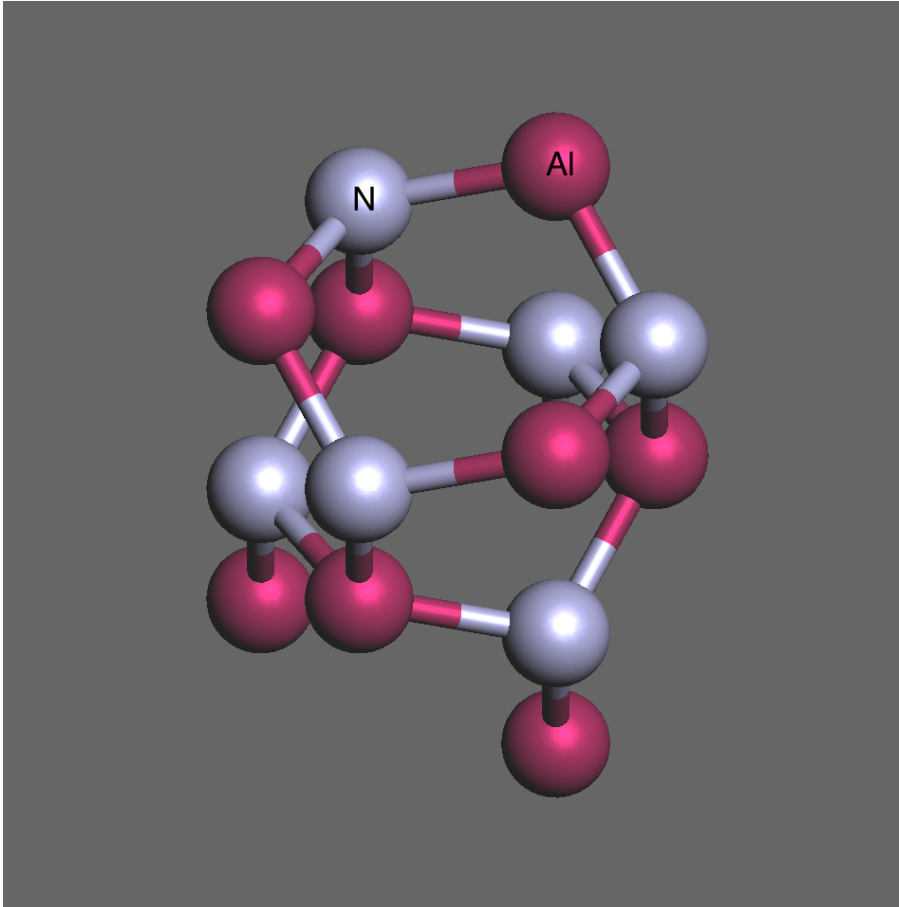
For each slice:

- **step 3:** calculate the projected potential: $(V_p(\vec{x}) = \frac{1}{c} \int_0^c V(\vec{x}, \zeta) d\zeta)$.
- **step 4:** calculate the diffractor: phase object function $(POF(\vec{x}) = e^{i\sigma V_p(\vec{x})})$.
- **step 5:** calculate the propagator $(e^{i\frac{k(\rho_1 - \rho_2)^2}{c}})$.
- **step 6:** stack the slices.
- **step 7:** iterate.

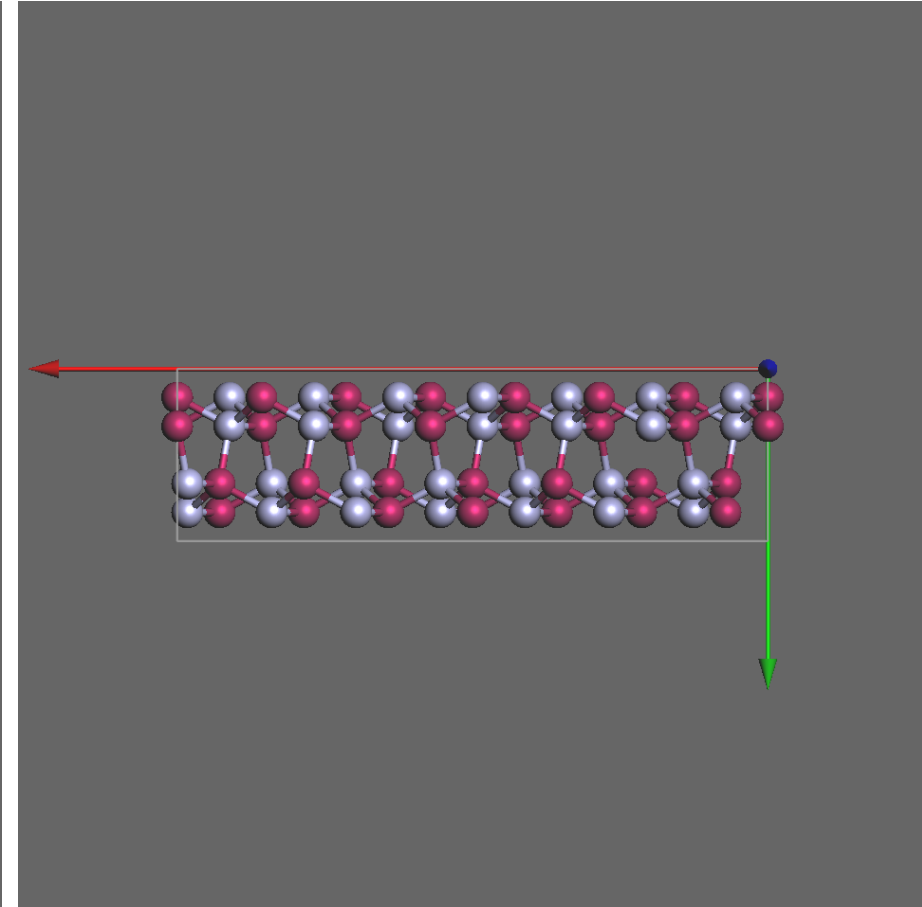


Multislice method: step 1 (AlN [1,1,1])

In order to define the slices (perpendicular to the optical axis), it is usually necessary to transform the crystal unit cell into an orthogonal cell (that can be pretty large).



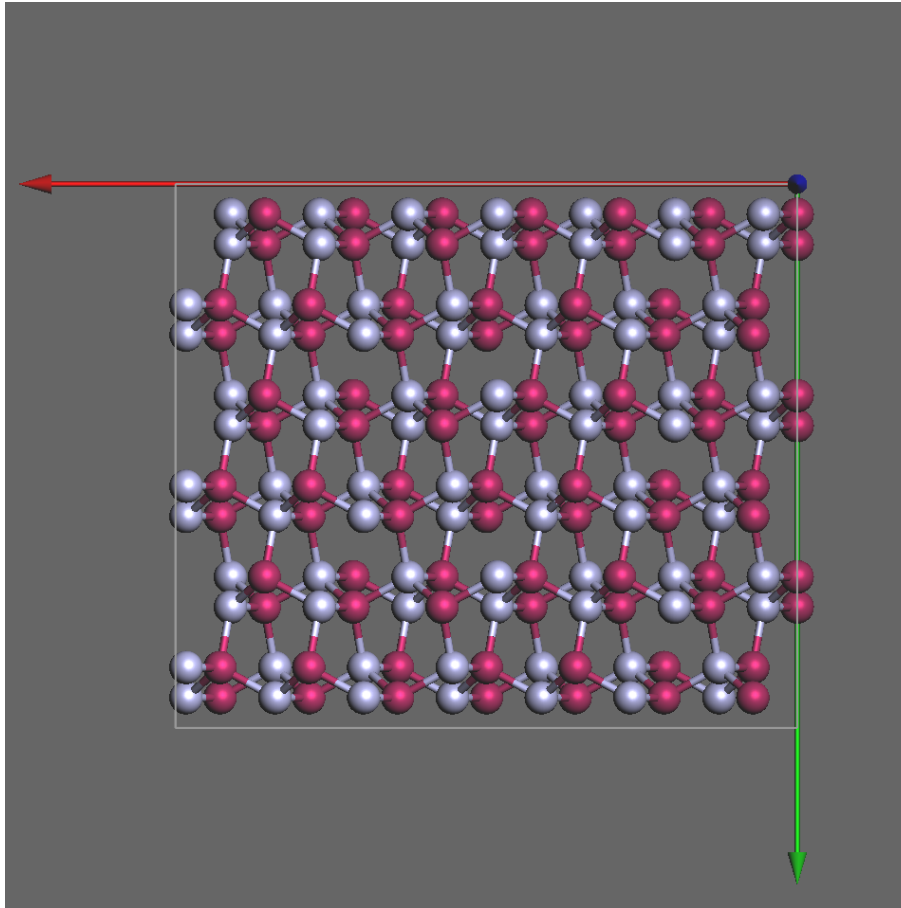
Model: AlN [1,1,1] projection (note the "square" groups of atoms).



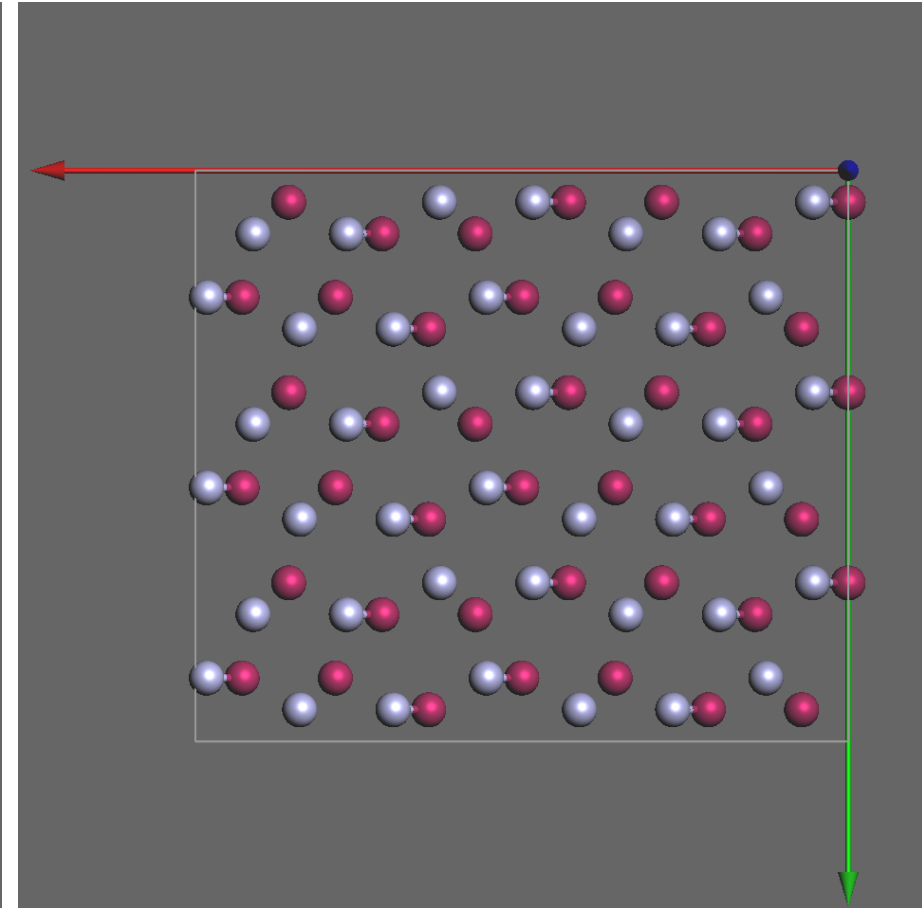
Transformed orthogonal AlN cell.

Step2: AlN [1,1,1] tetragonal slices

In order to define "*tetragonal*" slices (perpendicular to the optical axis), it is usually necessary to the orthogonal cell in order to make it more or less tetragonal (Fig. a). Finally the model is sliced (Fig. b).

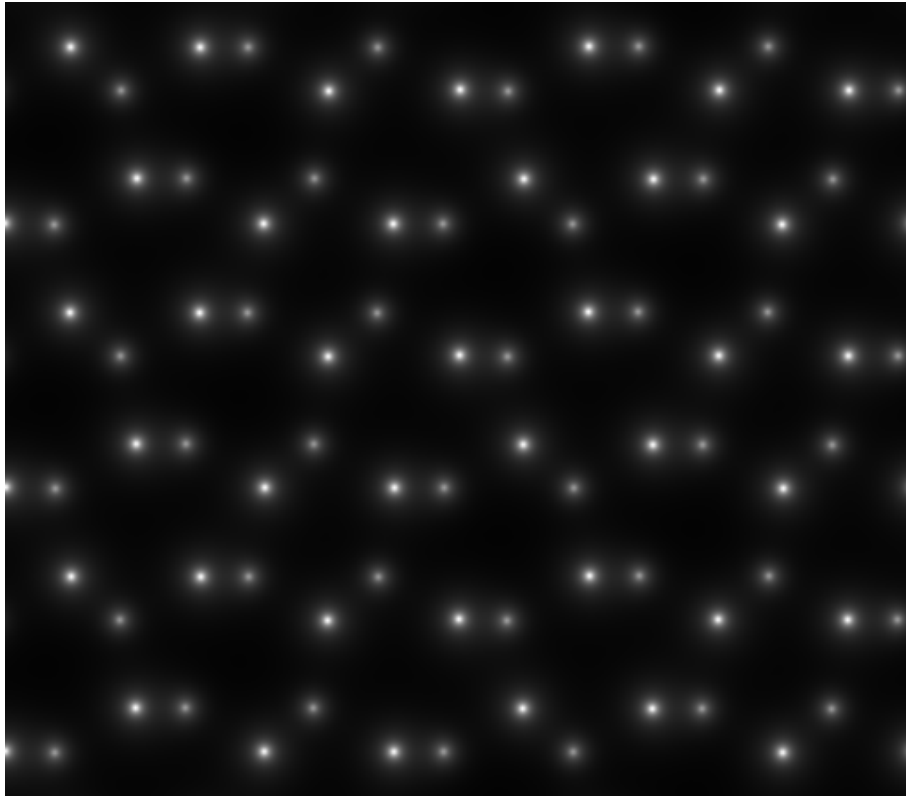


(a) AlN [1,1,1] orthogonal unit cell duplicated to (almost) tetragonal unit cell.

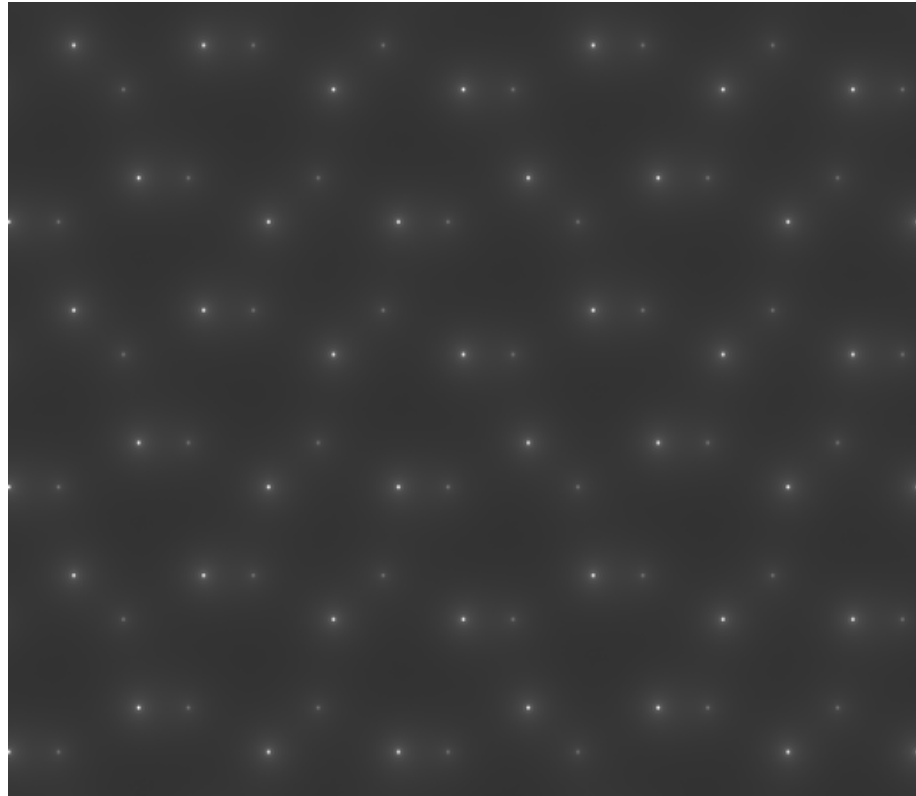


(b) AlN [1,1,1] this slice ready for multislice calculation.

Step 3: projected potential & TDS potential



Projected potential slice 1.

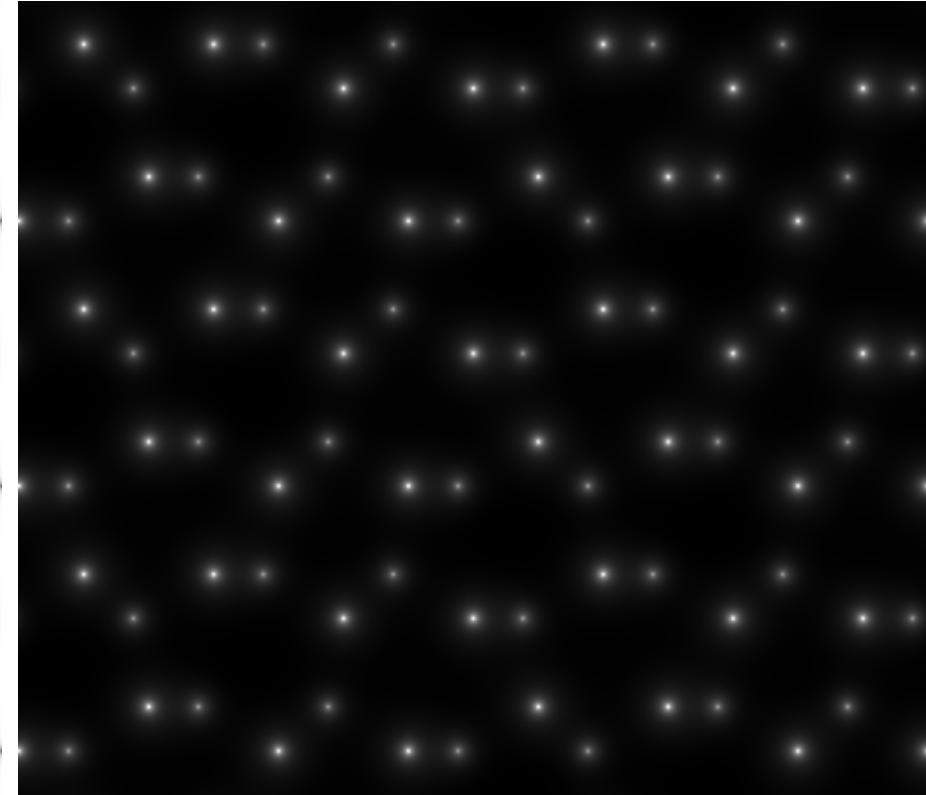


TDS potential slice 1.

Step 4: Phase object function: $POF(\vec{x})$

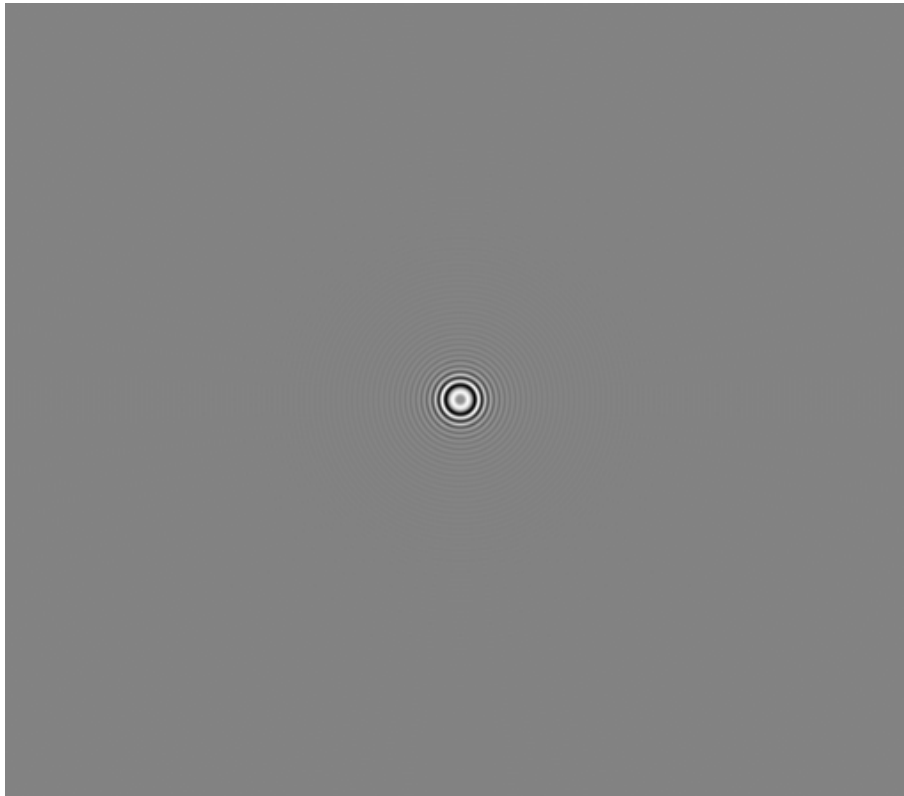


Phase object function slice 1 (real part).

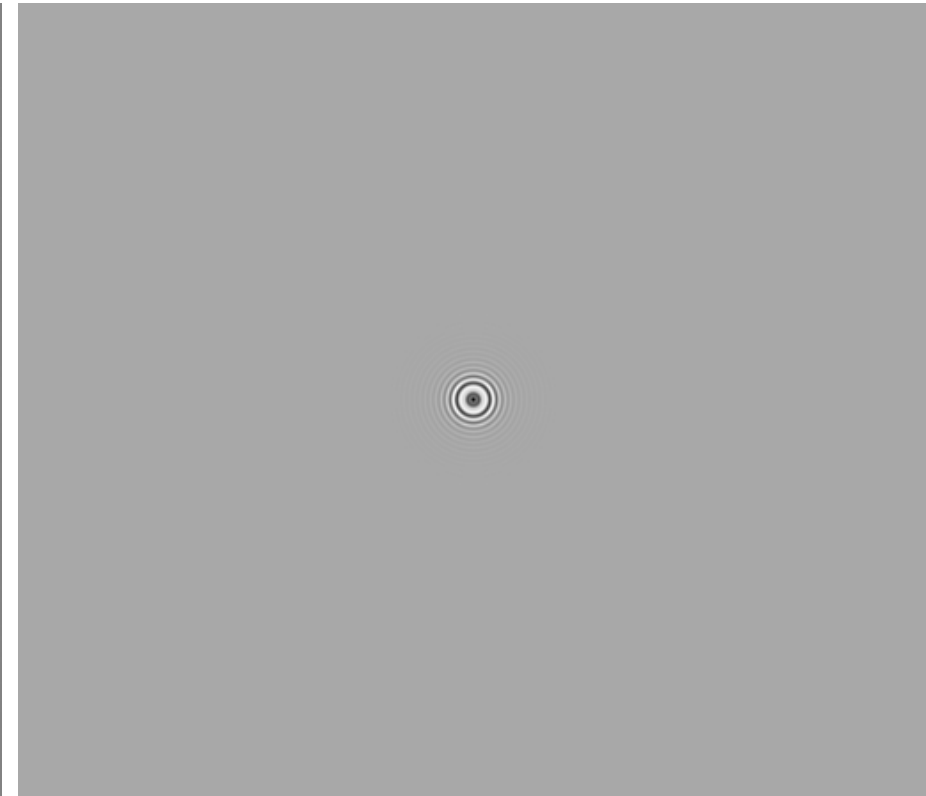


Phase object function slice 1 (imaginary part).

Step 5: Fresnel propagator: $FP(\vec{x})$



Fresnel propagator slice 1 (real part).



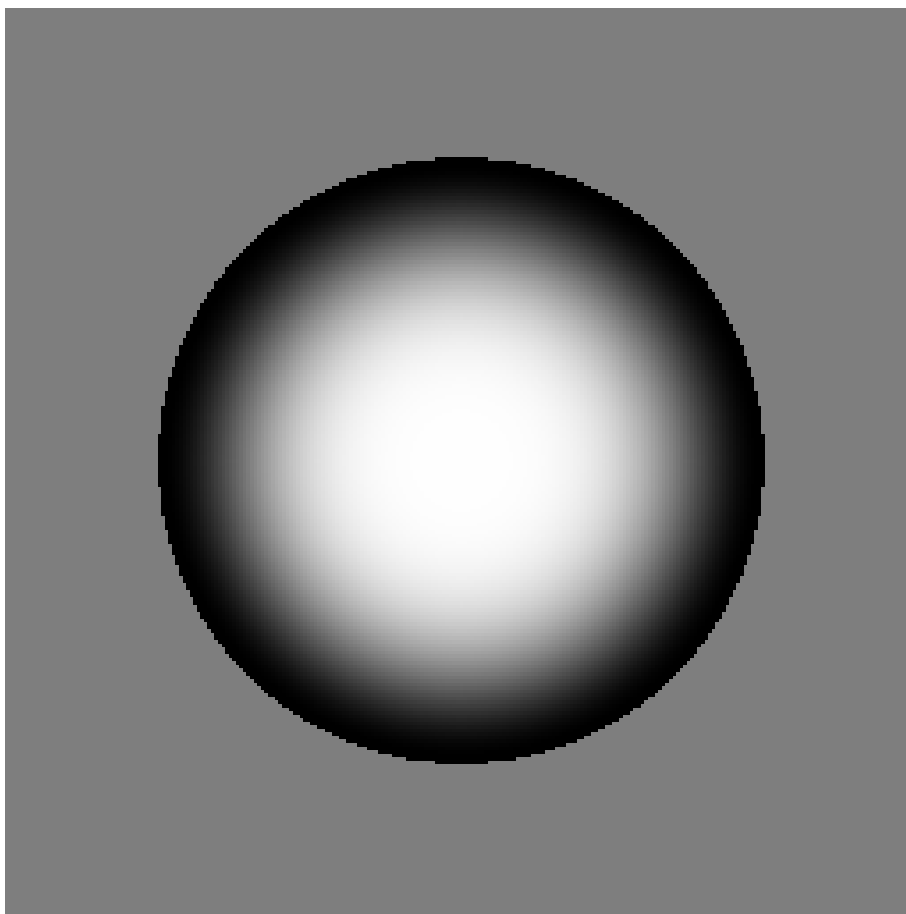
Fresnel propagator slice 1 (imaginary part).

Note: Diffraction in Fresnel approximation is a **convolution** of $f(\vec{x})$ (wave-function) after *slice*; with $g(\vec{x})$ (Fresnel propagator):

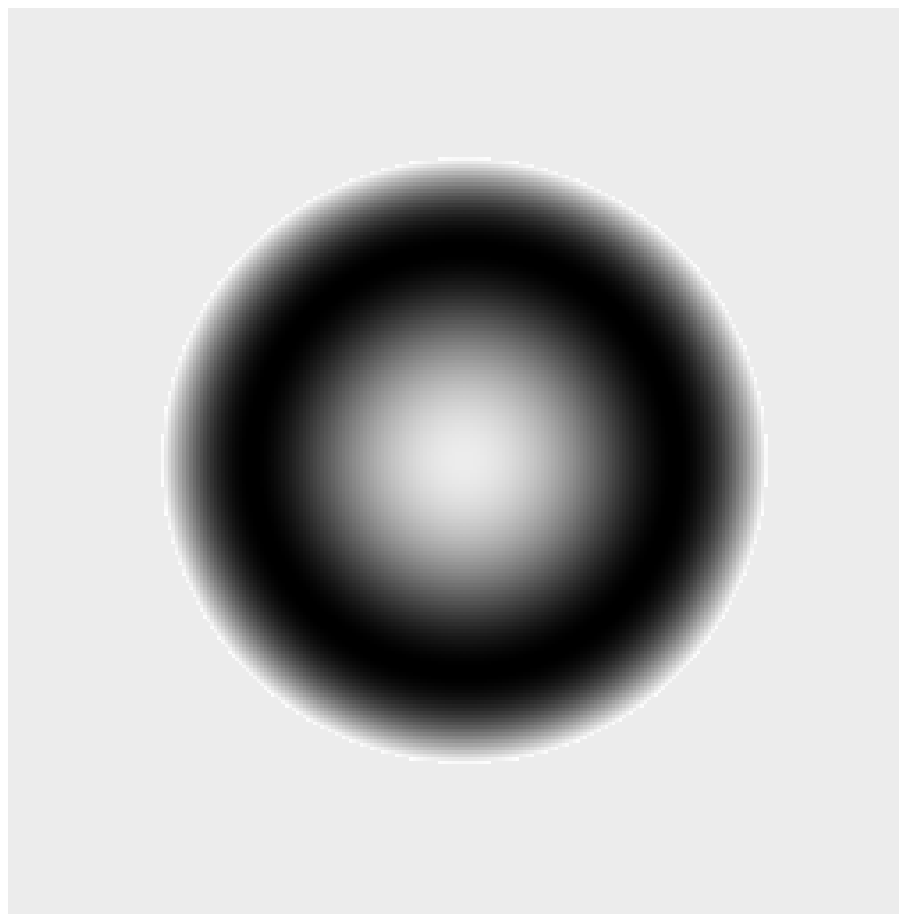
$$(f \otimes g)(\vec{x}) = \int_{-\infty}^{\infty} f(\vec{\tau})g(\vec{x} - \vec{\tau})d\vec{\tau} = \int_{-\infty}^{\infty} f(\vec{x} - \vec{\tau})g(\vec{\tau})d\vec{\tau}$$

Step 5: Fresnel propagator: $\widetilde{FP}(u, v)$

The convolution is usually performed in Fourier space:



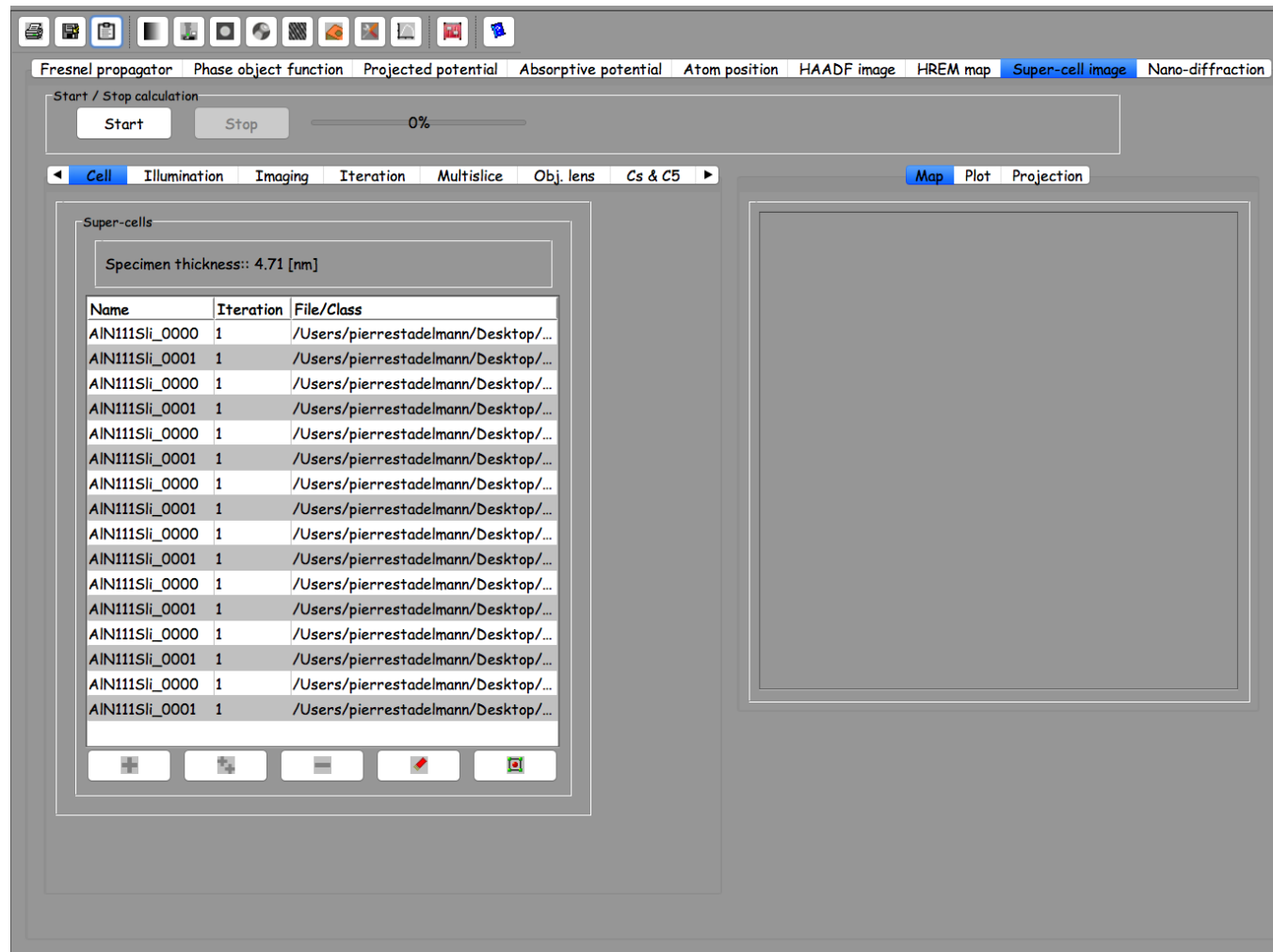
$FT\{\text{Fresnel propagator slice1}\}$ (real part).



$FT\{\text{Fresnel propagator slice1}\}$ (imaginary part).

$$(g \otimes h)(\vec{x}) = FT^{-1}\{FT\{g(\vec{x})\} \times FT\{h(\vec{x})\}\} = FT^{-1}\{\tilde{g}(\vec{u}) \times \tilde{h}(\vec{u})\}$$

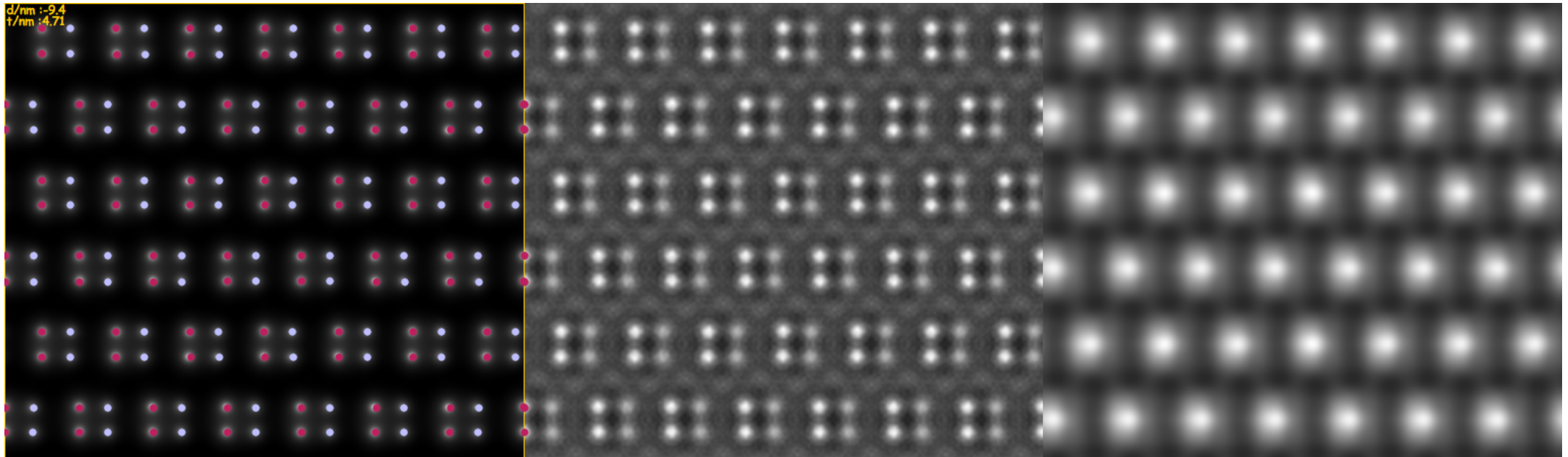
Step 6: prepare the stack of AIN [1,1,1] slices



Stack of AIN [1,1,1] slices.

Note: the slices do not have to repeat, they can all be different (but with identical lateral dimensions).

Step 7: do the multislice iterations



HRTEM AlN [1,1,1] (4.71 nm thick) (projected potential + atoms position, wave-function, image)

Wave-function after slice $n + 1$:

$$\Psi_{n+1}(x, y) = [\Psi_n(x, y) \otimes FP(x, y)] POF_{n+1}(x, y)$$

or:

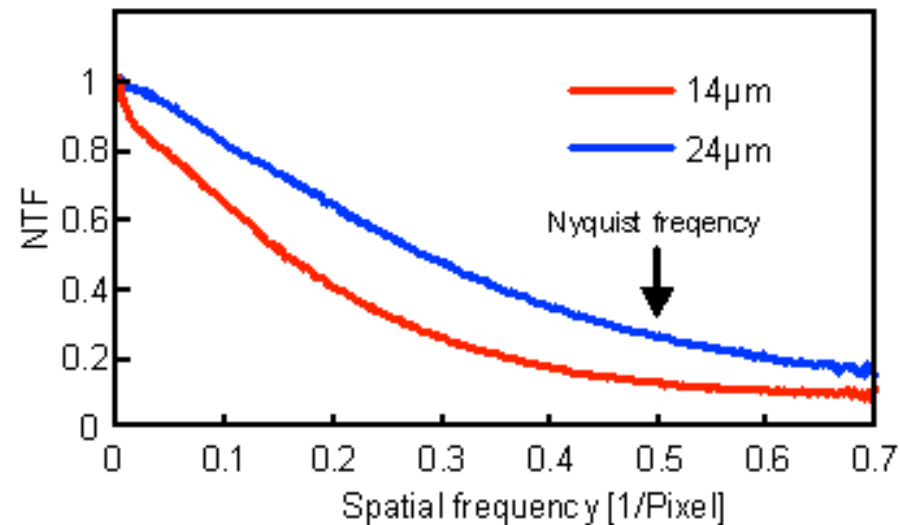
$$\Psi_{n+1}(\vec{x}) = [\Psi_n(\vec{x}) \otimes FP(\vec{x})] POF_{n+1}(\vec{x})$$

- ① Atomic model.
- ② Scattering and dynamical diffraction.
- ③ Image formation.
- ④ → **Image acquisition.**

Quantitative matching of simulated images against experimental micrographs is **not easy process**:

- First, it necessary to measure accurately the microscope and crystal parameters (i.e. aberrations, defocus, acc.voltage, coherence, vibrations, drift, crystal thickness and its precise orientation, etc) and to perform the images simulation using these measured values.
- Second, it is necessary to take into account the **Modulation Transfer Function** (MTF) of the **acquisition system** in order to match the **contrast** of experimental and calculated images.

The **transfer of intensity** by any acquisition system, in particular CCD cameras, is described by its MTF.

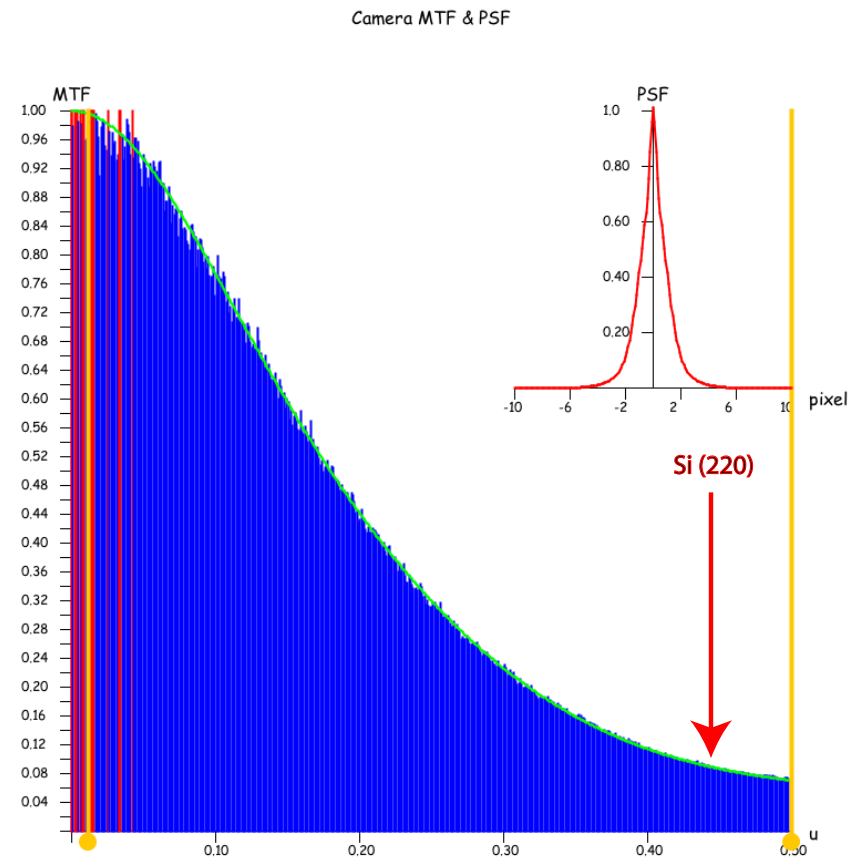
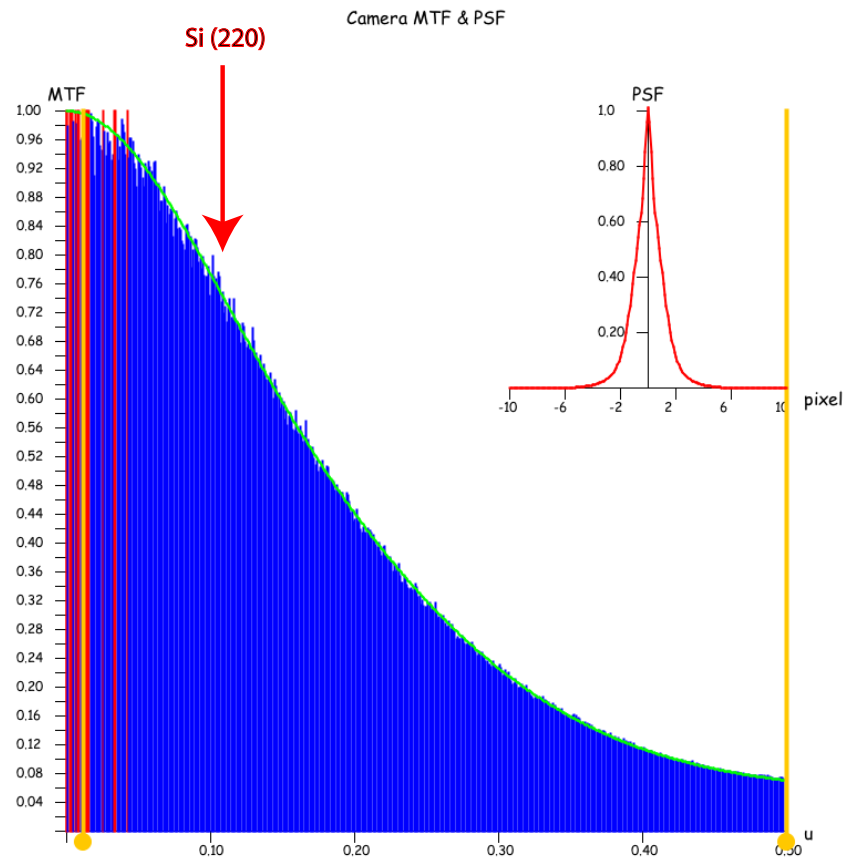


Noise transfer function (NTF) of 2k cameras with 14 µm and 24 µm pixel size (corrected for aliasing)

Comparison of the MTF of 2 CCD cameras. Note that the intensity of high spatial frequencies is severely attenuated.

Given a particular crystal, the contrast of the observed HRTEM micrographs depends on the TEM magnification. For quantitative work always record HRTEM micrographs at the highest possible magnification or introduce the detector MTF in the simulations.

MTF & Si (220) lattice planes

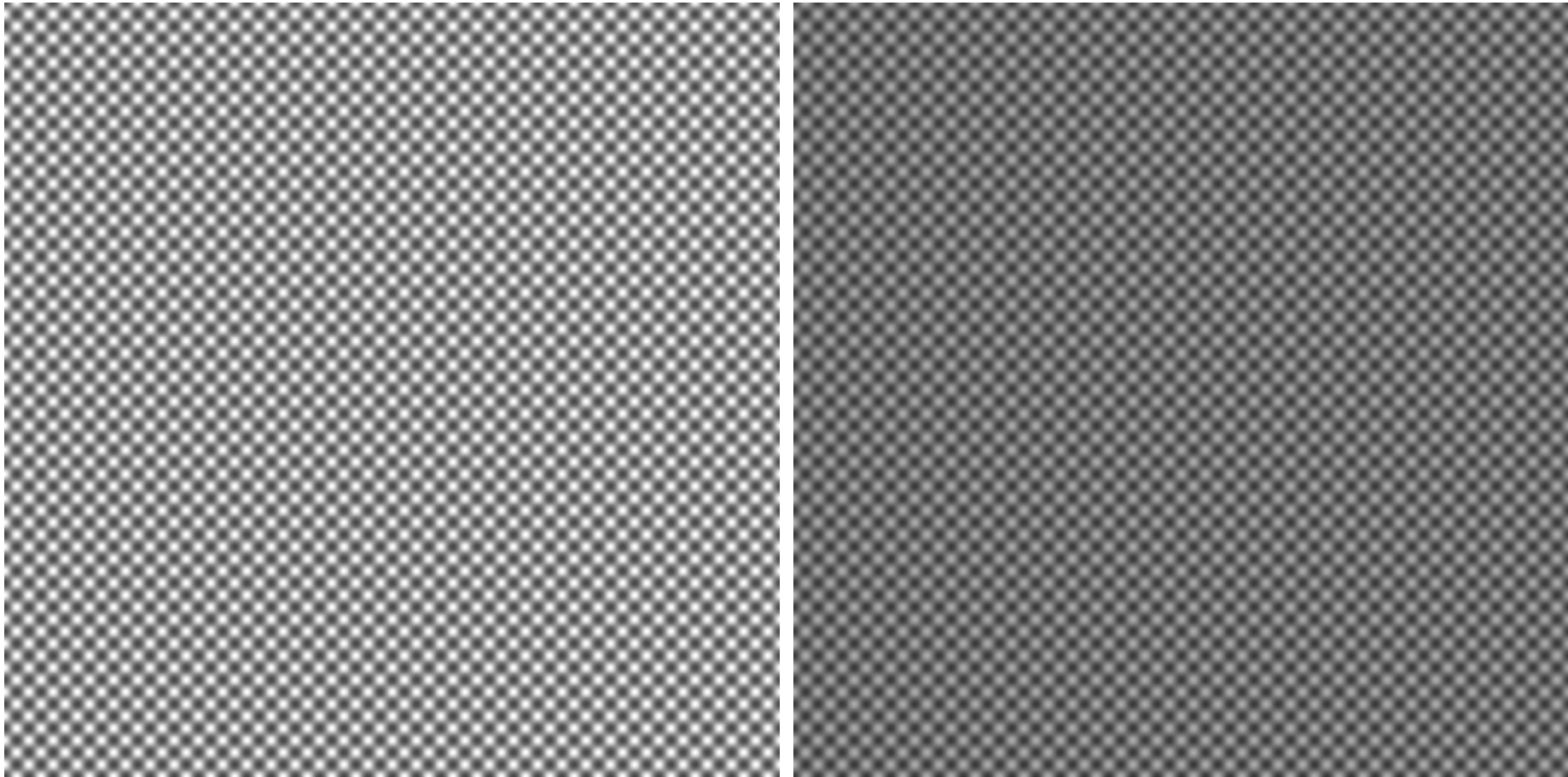


a: high magnification (preferred).
Few lattice planes on detector.
Good sampling → high contrast

b: low magnification.
Many lattice planes on detector
Bad sampling → low contrast

Si (220) spatial frequencies at high (a) and low (b) magnification (i.e. diffracted beams).

Effect of CCD MTF on simulated images: high magnification



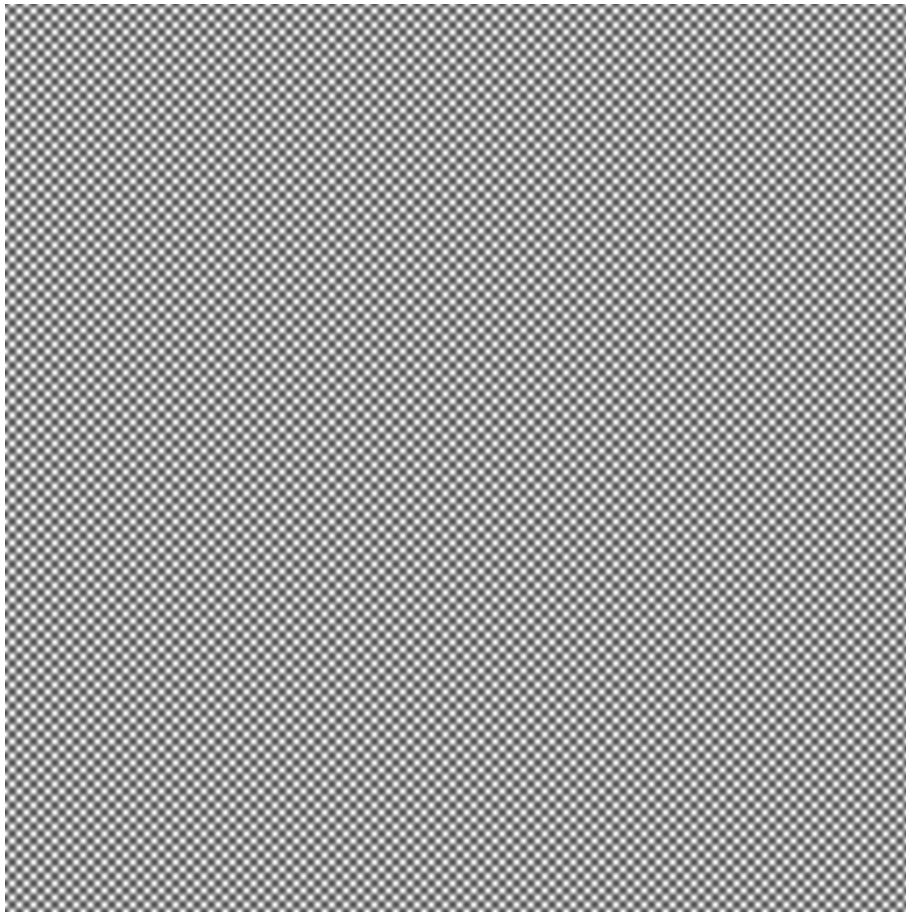
High magnification
CCD MTF **not included**.

High magnification
CCD MTF **included**.

At **high** magnification taking into account the MTF of the CCD camera reduces **significantly** the contrast of the simulated images (Stobbs effect!)².

²Experimental images can also be corrected to introduce the MTF of the detection system.

Effect of CCD MTF on simulated images: low magnification



Low magnification
CCD MTF not included.



Low magnification
CCD MTF included.

At low magnification the MTF of the CCD camera reduces drastically the contrast of the simulated images.

Please have jems installed on your PC or Mac before the labs. You can download the full jems program from the http address provided below (I can also provide jems on a USB key in case you can't download it).

You will have to request a license code (see installation instructions). The license code will be valid to December 31 2020.

- **jems documentation:** <http://www.jems-swiss.ch/>
- **jems executable:**
http://www.jems-swiss.ch/home/jemsv4_8431u2019.htm

3 versions are available for download:

- 1 **MacOS-X** 10.7 to 10.14.x (Mojave).
- 2 **Windows** 7 to 10.
- 3 **Linux ubuntu** 15.04 or later.