



Astigmatism [Å] / Coma / Coherence

	Mag.	Angle [°] w/horiz.
<input type="radio"/> Two fold	14	138
<input type="radio"/> Three fold	2873	97
<input type="radio"/> Coma	302	101

Sigma FWHM point spread Func. Å

Parameters (Left/Right Arrow keys adjusts)

- Microscope Focus [Å] Max Scatt. Angle: 324 mrad
- Probe Sampling [Å/px] Probe Rad: 12.8 Å
- # Sampling Points [px]
- Probe Semi-Angle [mrad]

All the parameters in the two dialog-sections define the probe and its shape. The aberrations are obvious input parameters and represent the microscope conditions. Under ideal circumstances the aberrations are all zero.

The point spread function is an empirical value that limits the resolution of the microscope as it smears out the data and eliminates the high frequency “noise” that originates in the calculation. It becomes a Gaussian low-pass filter as it convolutes the values at each pixel with a response function (Gaussian).

Based on the microscope parameters such as the voltage and spherical aberration, MacTempas sets the focus and the probe angle that optimizes the resolution (The later versions of MacTempas does this). The user is of course free to set the focus and probe angle that reflect the experimental setup.

The probe sampling sets the maximum frequency that is included in the calculation as is reflected by the max. scattering angle in milliradians. The size of the probe is a function of the number of sampling points and the actual sampling interval in Angstrom. One needs to make sure that the scattering angle is such that there are electrons being scattered onto the detector aperture.

The Detector aperture is again a function of the physical setup and should reflect this.

Detector Aperture

Dynamic (unchecking will reduce RAM needs)

Inner Aperture [mrad] 1.22 Å

Outer Aperture [mrad] 0.24 Å

Detector Aperture

Dynamic (unchecking will reduce RAM needs)

Inner Aperture [mrad] 1.22 Å

Outer Aperture [mrad] 0.24 Å

If the checkbox to the left “Dynamic” is checked, the program will output a new dialog window (see below) which will allow the user to see how the image vary as a function of the detector configuration (inner and outer apertures).

If the box is not checked, the output will be just a single image based on the fixed inner and outer aperture of the annular detector.

Output from STEM Calculation

Inner Aperture [mrad] 0.49 Å

Outer Aperture [mrad] 0.15 Å

Double click in image to make it display in separate image window

Thickness [Å]

Save Current Image...

Save Current Image Stack as MRC file...

Image # - of -
From: - To: - mrad

Current STEM Image as a function of Inner and Outer Detector Radii

ImageStack: Images as a function of reciprocal scattering angle

Specimen

Scan Increment [px]
Image Sampling 0.250 Å/px

Use Frozen Phonon Model

Number of configurations
 Show average potential for config.

Subslice potential
Unit Cell Divided into Slices

Show potential for each slice

As the sampling needs to be fine enough so that the calculation extend to high g -values (scattering angles), it gives a better resolution than what the microscope is capable of (hence the point spread function introduced earlier). Thus the specimen does not need to be sampled at the same interval. In this case, the specimen is only sampled at every 5 points of the sampling of the potential.

In order to smooth out the data (the image), the calculated image is oversampled. The oversampling of the image, combined with the point spread function result in a smooth image at a resolution reflecting the actual resolution of the microscope. Of course one has to be careful not to sample too coarsely.

The output image is given a dimension of N by M times the unit cell used for the calculation. The unit cell used in the calculation should be the smallest repeat cell as anything greater just increases the calculation time unnecessarily.

STEM Image

oversample output image X

Cells Wide High

Image Size 420 by 420

Rectangular Image (oblique unit cells)

Specimen

Scan Increment [px]

Image Sampling 0.250 Å/px

Use Frozen Phonon Model

Number of configurations

Show average potential for config.

Subslice potential

Unit Cell Divided into Slices

Show potential for each slice

This setting determines how the potential is calculated. The lower checkbox and subsequent value set how many slices the unit cell is divided into.

If the option “Use Frozen Phonon Model” is checked, all the atoms in each slice will be randomly displaced following a gaussian distribution with a sigma reflecting the debye-waller factor of the atom(s). The number of configurations will set how many times the multi-slice calculation is performed for the given thickness. Each time, the atoms in every slice is displaced ; each time a new image is produced. At the end, the images are all added up (for each configuration) to produce the final image.

Clearly, the calculation time increases as the number of configurations increases. Likewise it is more time consuming to displace atoms and calculate new potentials for every slice. One has to realize that a full multi-slice calculation for the total thickness is performed for every sampling point of the specimen.