# ImageSim-TEM tutorial

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## **HRTEM Image Simulation**

🚽 qstem	
Select a complex wave function	
Look in: 🗀 2_v=+0-5 💌 🖛 🖭 -	Simulate images from wave function
STO_110_68.ing	
STO_110_59.img B wave_2.img	Probe array
STO_110_Proj.img wave_4.img wave_5.img	
a wave_0.img wave_6.img	
	Scattering angle: 124.843 X 127.335 Images from wave
Filename: wave Sing	
	Number of horizontal model sub-stabs: 1
Files of type: Wave function	Number of slices per sub-slab: 20 POPTUP WINDOW
	Slice thickness: 0.2725 A
0 5 10 13 20	Center slices Periodic X,Y Periodic Z
2. Select folder	
where wave	Microscope parameters       High voltage:       200       kV       (wavelength = 2.51pm)
	Defocus:60 nm Scherzer
functions are saved	Astigmatism: 0 nm, angle: 0 deg
– select wave	Spherical Aberr. C3: 1.0 mm
View from	Temperature: 300 K, TDS runs: 30 V TDS
Load Model Update View 3D C Unit cell C top	Cc: 1.0 mm, dE: 0.5 eV
Model Properties size 50 C Super cell Front	Convergence angle: 15 mrad
Unit cells: Nx: 1 Ny: 1 Nz: 1 C Box C Ncell	Detectors:     Dumber: 1 + Inner angle: 70 Outer angle: 200 mrad
Sample tilt: X: 0 Y: 0 Z: 0 Odeg Orad	Auto Data Offset Y: The Offset Y: The Offset Y:
C STEM © TEM	Slices between outputs: 10 Folder: test
Load Config         Save Config         Advanced Settings         Start Simulation         Display R	esults

## **Enter TEM parameters**





#### **Thickness-Defocus Series**



Select the different thicknesses – these are the output wave functions from the simulation done previously.

Select wave functions from which you want to simulate defocus series (in most cases wave functions at different [intermediate] sample thicknesses, but can also be wave functions for different frozen phonon configurations, or both).

#### **View Results**

Load Model       Update View       3D       Z size         Model Properties       size       50       Unit cell         Model Properties       size       50       Super cell       Image: front         Unit cells:       Nx:       1       Ny:       1       Nz:       1       Box       Ncells         Sample tilt:       X:       0       Y:       0       Z:       0       Image: deg constraints         Simulation mode       Image: Step Step Step Step Step Step Step Step	Convergence angle:       15       mrad         Detectors:
1. From main window - click "Display Results" to open pop up window	2. Click "Select Folder", opens a new pop-up window
Alternatively, one can also import the images into DigitalMicrograph	Showimage     File     1     0.9     0.9     0.9     Select folder     img     Stopms   Stopms   Stopmation     Stopmation     Stopmation     Stopmation     Stopmation     Stopmation <tr< th=""></tr<>
3. Select the folder location where the wave functions or images are located	SIO_ms_Tilt_neg2_neg5_mrad         STO_ms_Tilt_neg5_neg2_mrad         STO_Tilt_2_5_mrad         Tem ExampleClass         New Folder         New Folder         Make New Folder         OK         Cancel