Manual of ToTEM Software

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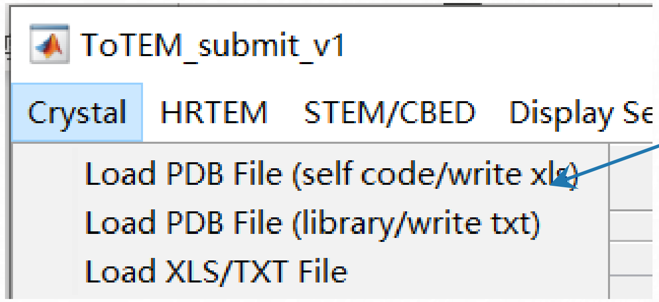
CONTENT

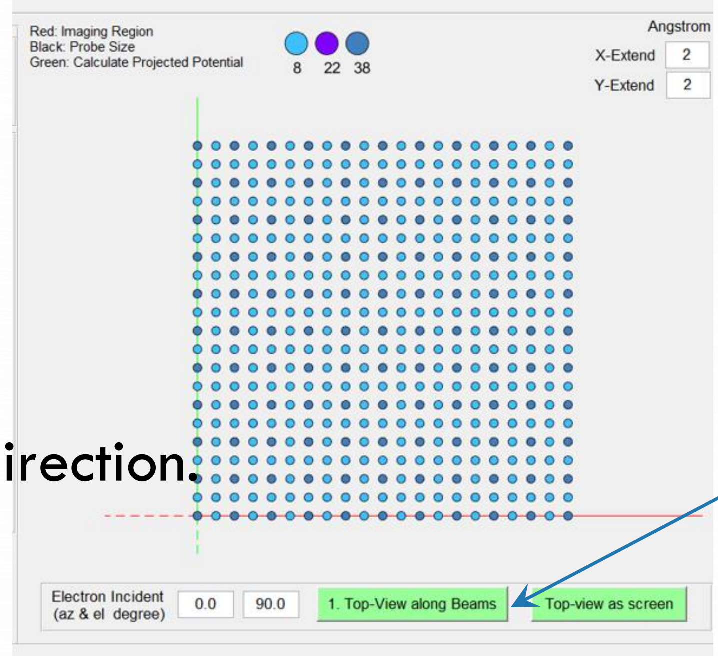
I. QUICK OPERATION

0. Run mex_cuda.m and then ToTEM_submit_v1.m (source code).



Anyone of three

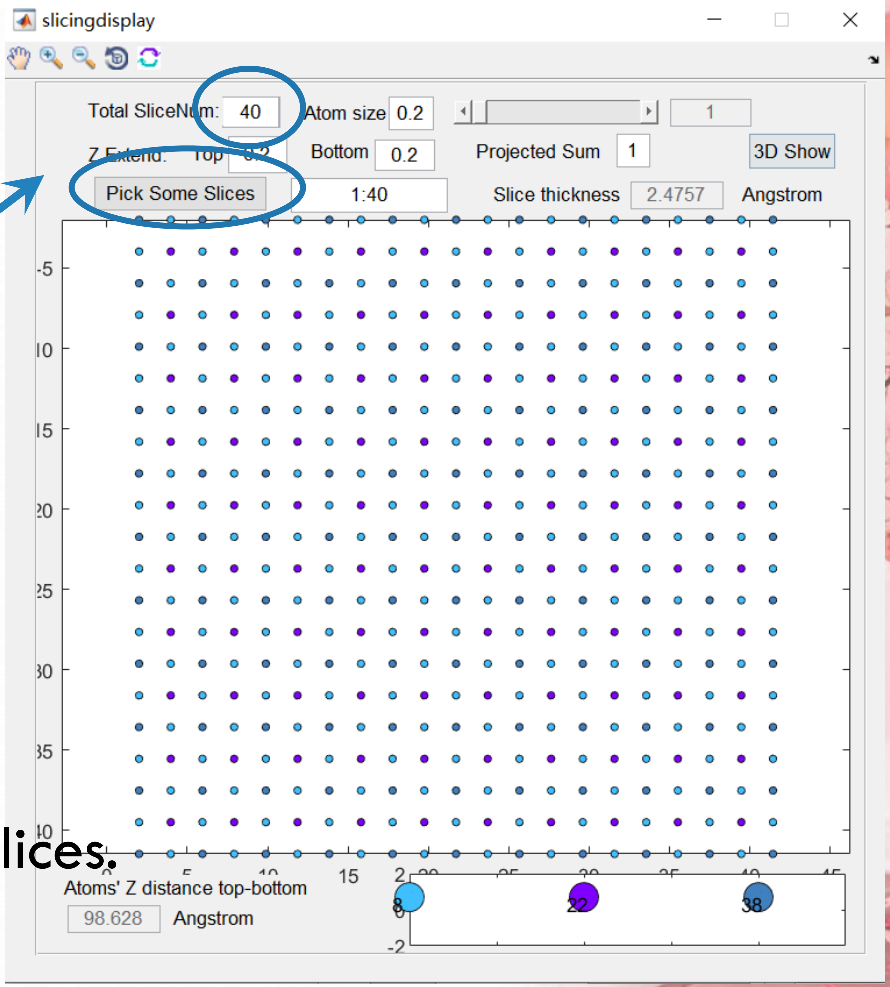
1、 Read information about a supercell.



2、 Press radio button to get a special direction.

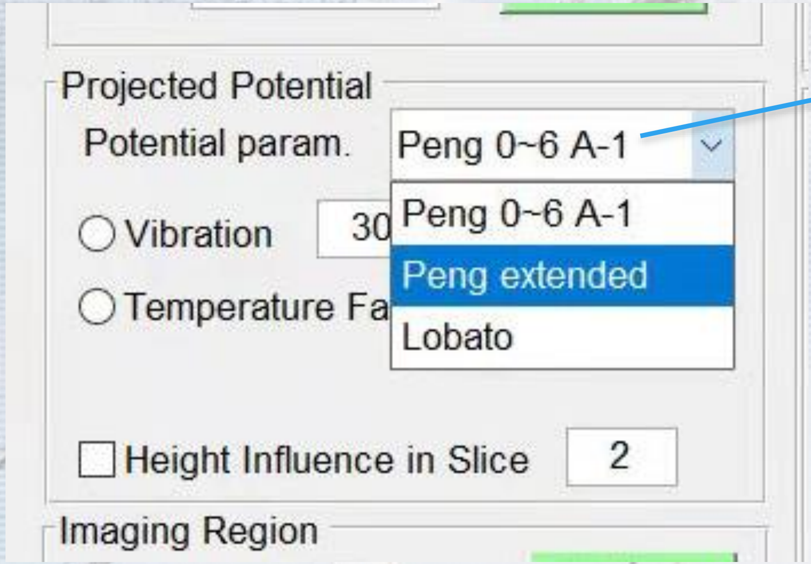
Anyone of two

3a、 Slicing crystal by pressing ‘Slicing’ radio button to control a sub-dialog.



3b. Set the total slice number and pick some slices.

4、Selection for atomic scattering factor and vibration. For example:

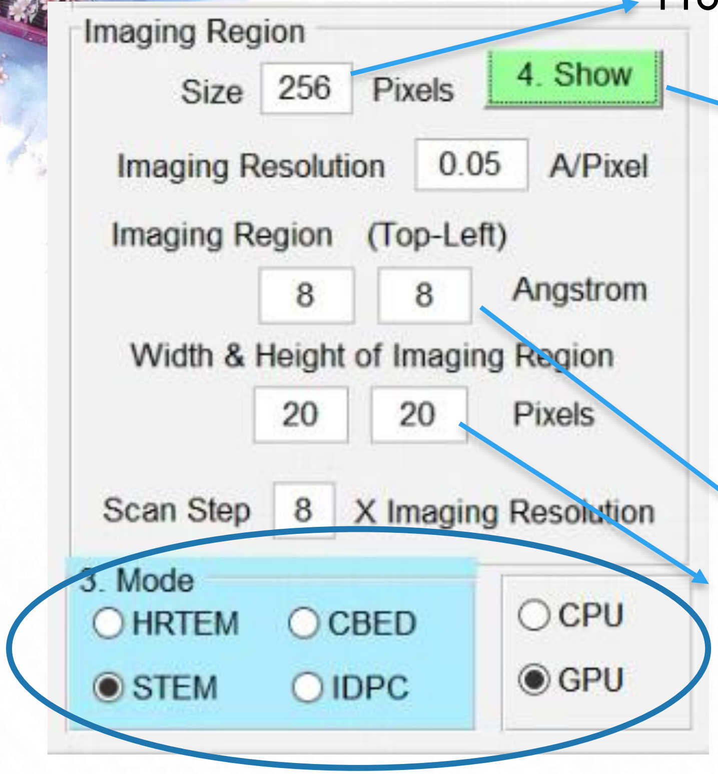


select atomic scattering factor

Choose whether to consider vibration or temperature factor, whether to assign potential into multiple slices.

5a、 Select STEM/HRTEM mode and set region and parameters. A STEM example:

Probe size

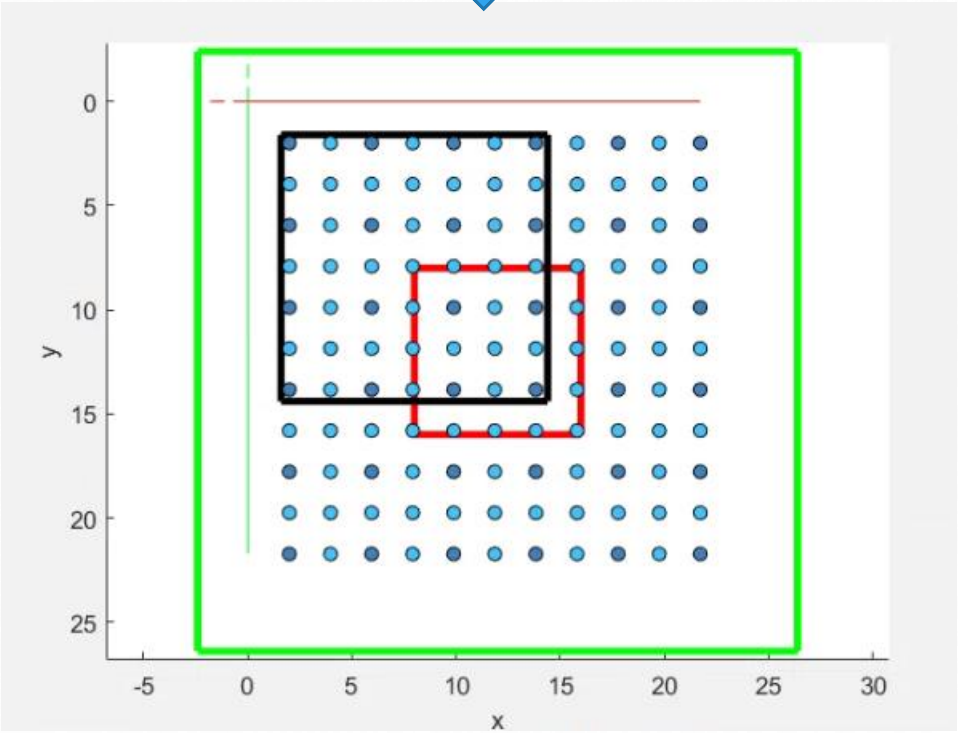


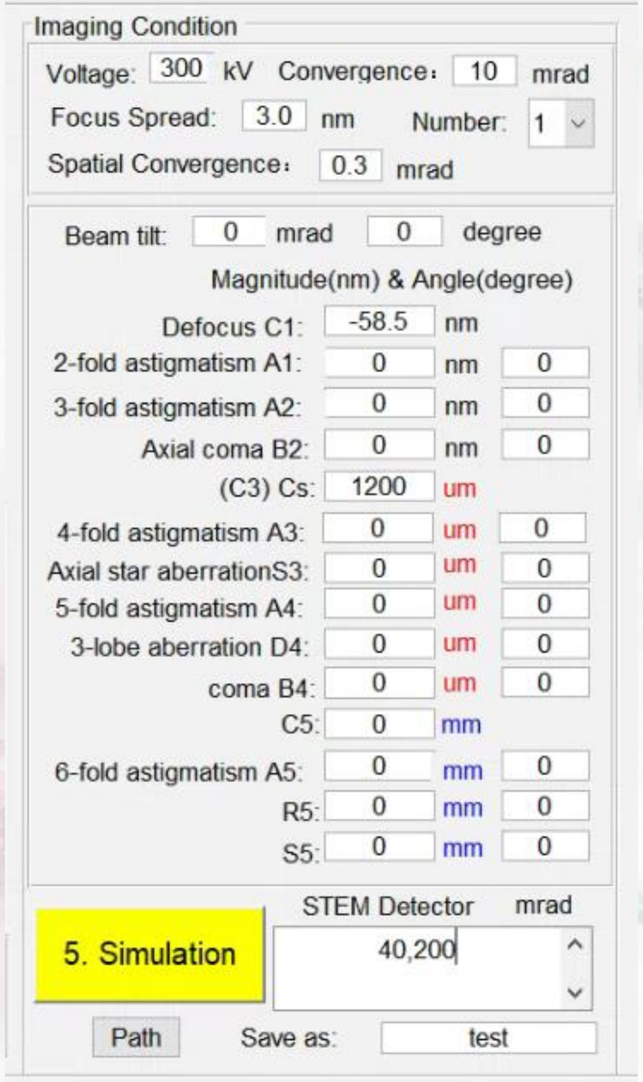
You must click this button when you're done

Image starting position

Image size

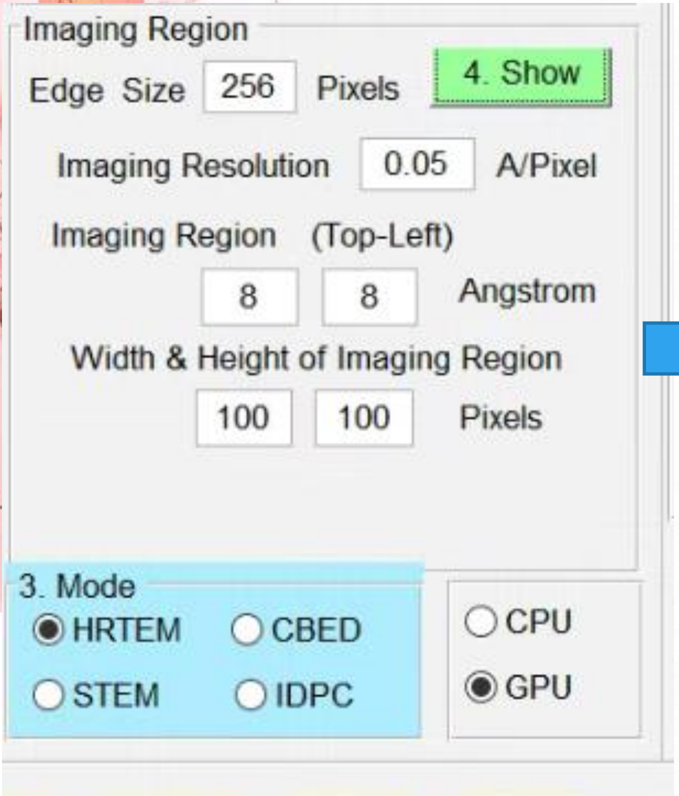
Imaging area

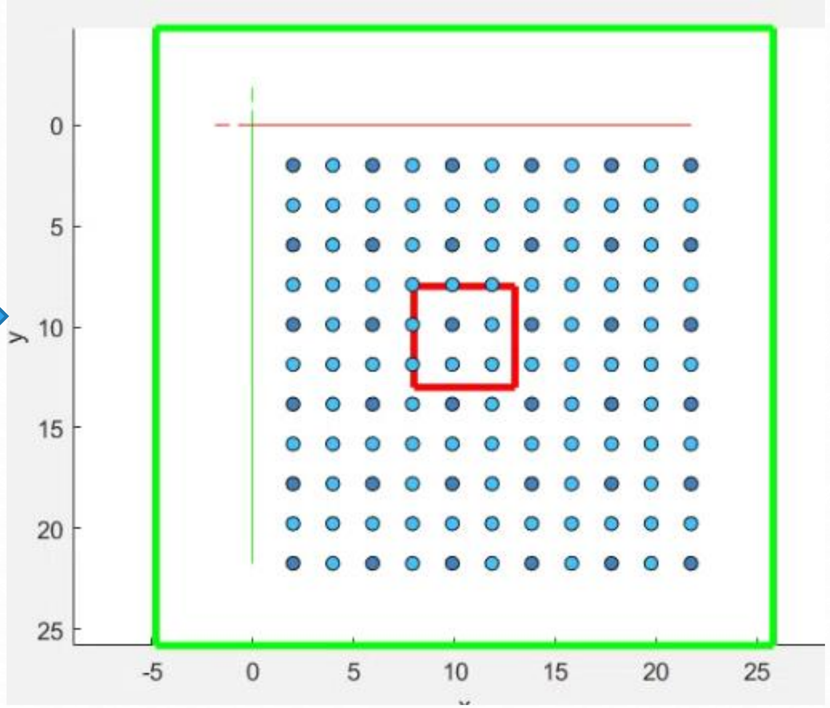


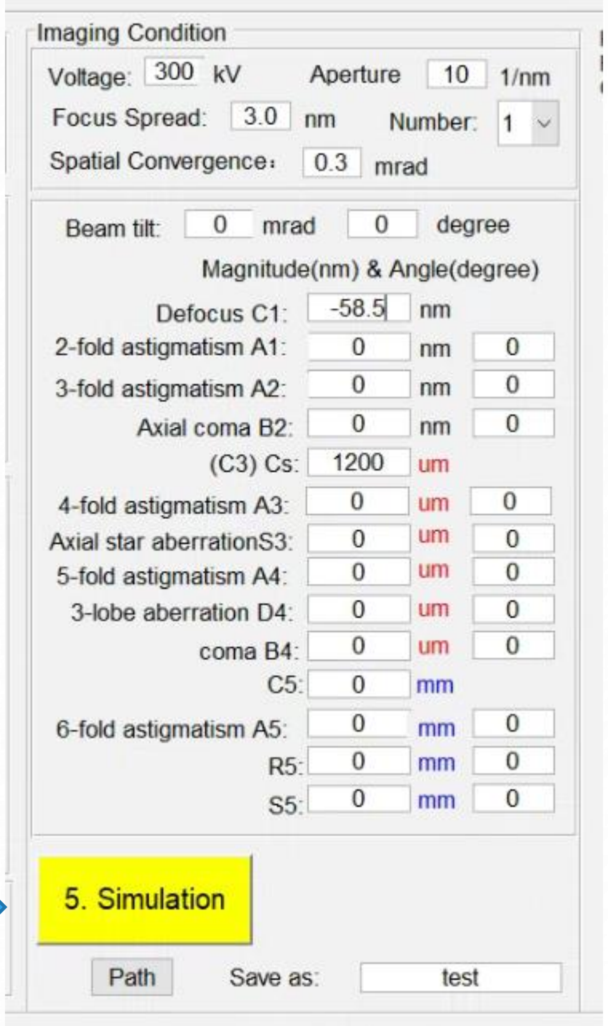


Other Parameter Settings and simulation.

5b、Select STEM/HRTEM mode and set region and parameters. A HRTEM example.







II. ENVIRONMENT CONFIGURATION

1. Installer

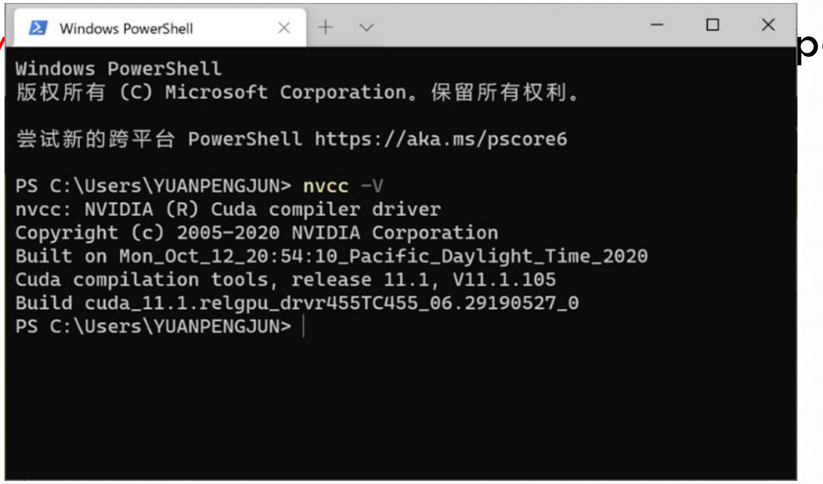
You can run this software on Windows or Linux with or without a CUDA environment. Here's how to run it on Windows and Linux (Ubuntu) with a CUDA environment.

Run mex_cuda.m first!

1.1 WINDOWS

1.1.1 CUDA

Open https://developer.nvidia.com/cuda-dow pe 'nvcc-v' at the terminal.
Installation is successful if display as Fig. 1-1,



1.1.2 MCR

Open https://www.mathworks.com/products/compiler/matlab-runtime.html to install the 'MATLAB Runtime Version 2020b (9.9) Version'. Please choose the version on 'Windows 64-bit'.

1.1.3 RUN

Double-click 'ToTEM.exe' to run it.

1.2 Ubuntu

1.2.1 CUDA

Open https://developer.nvidia.com/cuda-downloads to install 'cuda 11 version', Then type 'nvcc-v' at the terminal. If the terminal has CUDA 11 version information, installation is successful.

1.2.2 MCR

Open https://www.mathworks.com/products/compiler/matlab-runtime.html to install the 'MATLAB Runtime Version R2019b (9.7) Version' of 'Linux 64-bit'.

1.2.3 RUN

Type './run_ToTEM.sh <mcr_directory> at terminal to run it. For example, if you have version 9.9 of the MATLAB Runtime installed in the folder: '/mathworks/home/application/v99', run the shell by using this script,

```
./run_ToTEM_v3.sh /mathworks/home/application/v99
```

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III. DETAILS

- **0. GUI**
- **1. Import a crystal**
- **2. Slicing dialog of multislice method**
- **3. Parameter settings about simulation**
  - 3.1 Vibration, DW factors and absorption
  - 3.2 Imaging region
  - 3.3 Coherence
  - 3.4 Lens parameters
  - 3.5 Detector’s angle format
- **4. Other functions**
  - 4.1 CPU/GPU parallels
  - 4.2 HRTEM related
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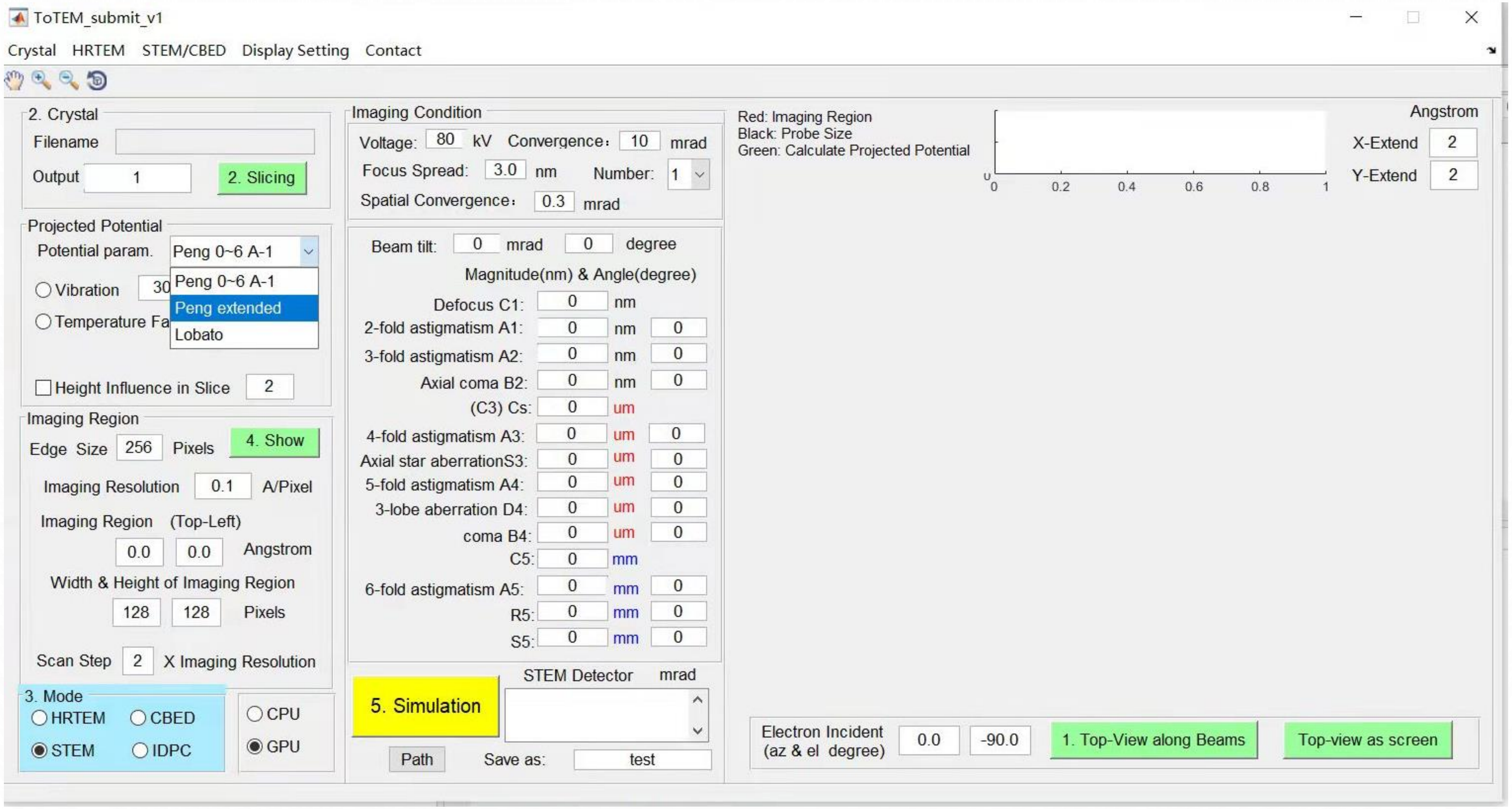
- **5. Examples**
  - 5.1 HRTEM
    - 5.1.1 HRTEM Simulation for one single image
    - 5.1.2 Batch Simulation
  - 5.2 CBED
  - 5.3 STEM
  - 5.4 IDPC
  - 5.5 IDPC Simulation for MFI-type zeolites

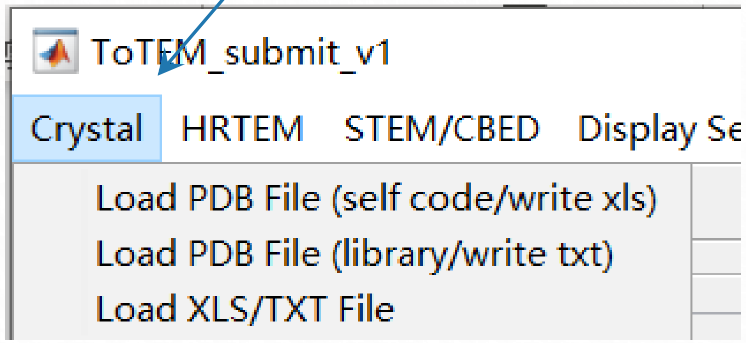
0. GUI



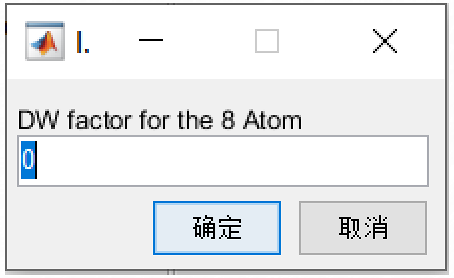
ToTEM_submit_v1
Crystal
HRTEM
STEM/CBED
Display Setting
Contact
2. Crystal
Filename
Output
1
2. Slicing
Projected Potential
Potential param.
Peng 0~6 A-1
Peng 0~6 A-1
Peng extended
Lobato
Vibration
30
Temperature Fa
Height Influence in Slice
2
Imaging Region
Edge Size
256
Pixels
4. Show
Imaging Resolution
0.1
A/Pixel
Imaging Region (Top-Left)
0.0
0.0
Angstrom
Width & Height of Imaging Region
128
128
Pixels
Scan Step
2
X Imaging Resolution
3. Mode
HRTEM
CBED
STEM
IDPC
CPU
GPU
Imaging Condition
Voltage:
80
kV
Convergence:
10
mrad
Focus Spread:
3.0
nm
Number:
1
Spatial Convergence:
0.3
mrad
Beam tilt:
0
mrad
0
degree
Magnitude(nm) & Angle(degree)
Defocus C1:
2-fold astigmatism A1:
3-fold astigmatism A2:
Axial coma B2:
(C3) Cs:
4-fold astigmatism A3:
Axial star aberrationS3:
5-fold astigmatism A4:
3-lobe aberration D4:
coma B4:
C5:
6-fold astigmatism A5:
R5:
S5:
nm
um
mm
5. Simulation
STEM Detector
mrad
Path
Save as:
test
Red: Imaging Region
Black: Probe Size
Green: Calculate Projected Potential
0
0.2
0.4
0.6
0.8
1
Angstrom
X-Extend
2
Y-Extend
2
Electron Incident
(az & el degree)
0.0
-90.0
1. Top-View along Beams
Top-view as screen

1. Import a crystal

Import crystal information from a PDB file or an excel or text file.



Input Debye-waller (DW) factor for every element. The dialog box will pop up after importing a PDB file



A *.xls or *.txt file will be generated after reading a pdb file.
Next time you can import it without inputting DW factors.

Information in a xls or txt file.

Atomic number

Coordinators (units: Å)

Valence state

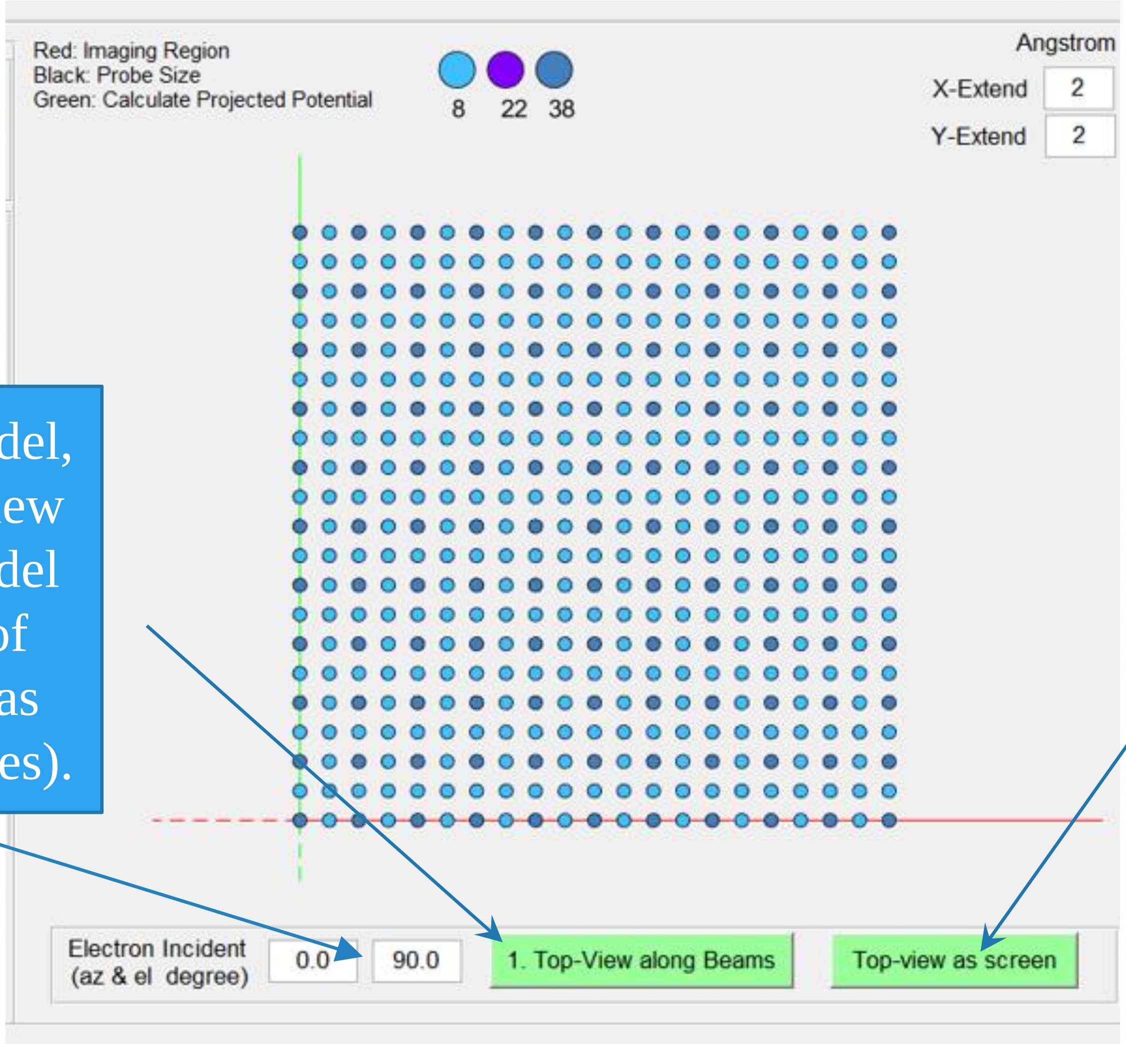
Ionicity

temperature

Occupancy rate

	A	B	C	D	E	F	G	H
1	8	-1.973	0	-1.973	0	0	0.7875	1
2	8	-5.918	0	-1.973	0	0	0.7875	1
3	8	-9.863	0	-1.973	0	0	0.7875	1
4	8	-13.808	0	-1.973	0	0	0.7875	1
5	8	-17.753	0	-1.973	0	0	0.7875	1
6	8	-21.698	0	-1.973	0	0	0.7875	1
7	8	-25.643	0	-1.973	0	0	0.7875	1
8	8	-29.588	0	-1.973	0	0	0.7875	1

You can conveniently edit it via other tools.



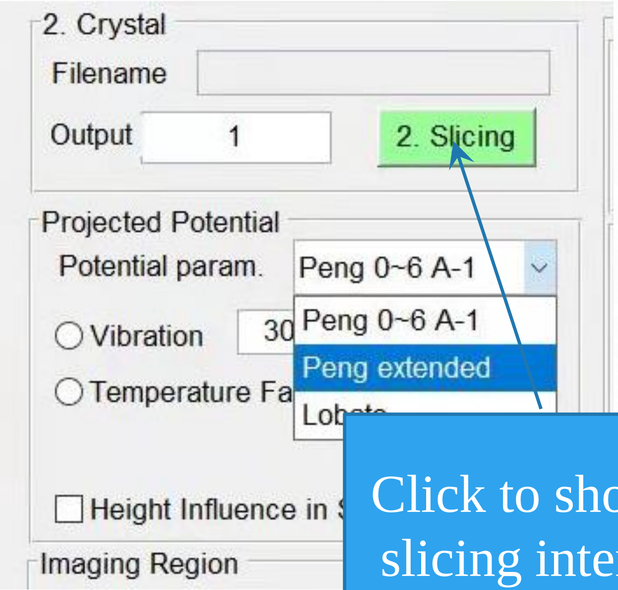
After importing a model, click this button to view and calculate the model from the direction of electron incidence (as values in the edit boxes).

Or you can see the model from any angle after mouse rotating.

Note: at least one button must be clicked

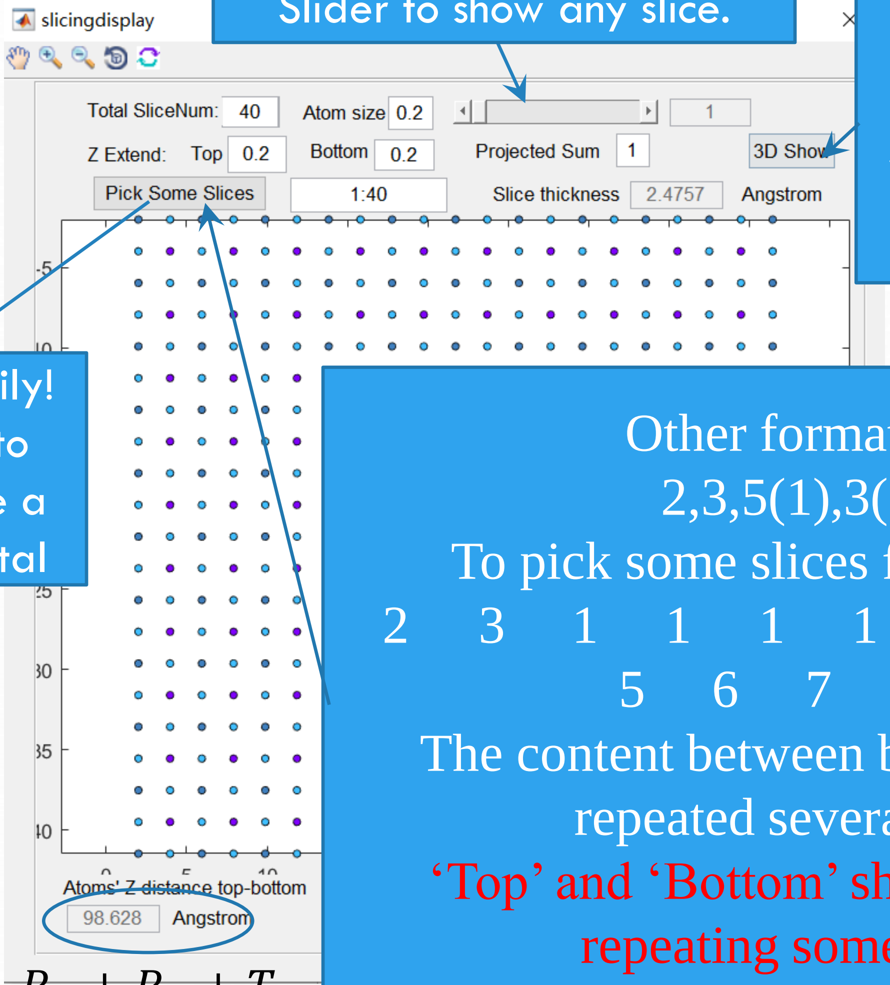
2.Slicing dialog of multislice method

If some atoms were lost after slicing, please add a very small vacuum on top or bottom, such as 0.00001.



Click to show the slicing interface.

Slider to show any slice.



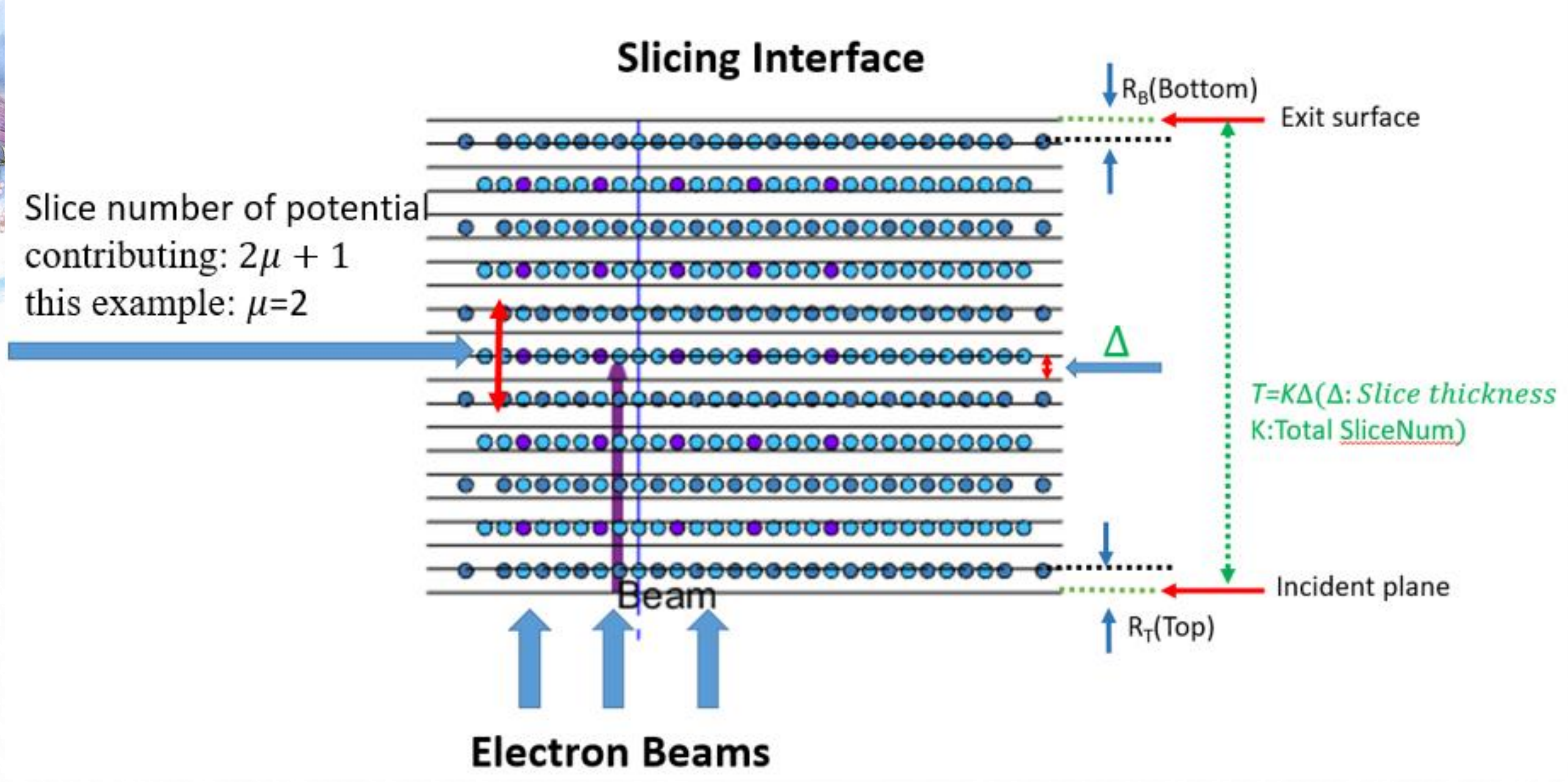
$R_T + R_B + T$

After setting the slicing parameters, you must click the button to display the slicing results.

Necessarily! Click it to generate a new crystal

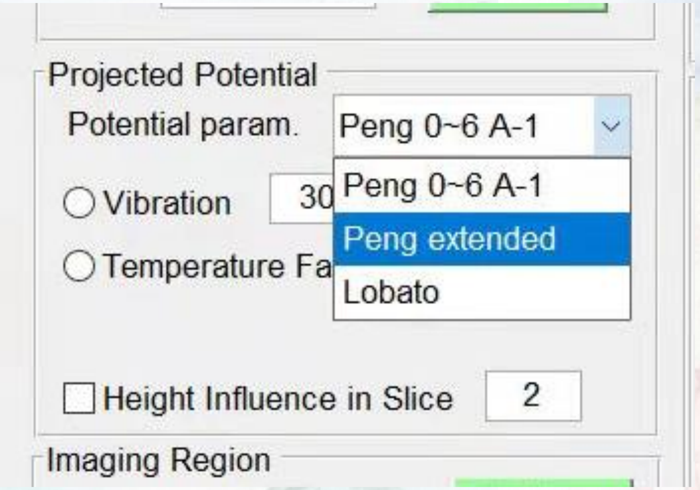
Other format like:
2,3,5(1),3(5:7)
To pick some slices from all slices
2 3 1 1 1 1 1 5 6 7 5 6 7 5 6 7
The content between brackets will be repeated several times.
'Top' and 'Bottom' should be zero if repeating some slices!

Slicing result



3. Parameter settings about simulation

3.1 Vibration, Temperature Factors

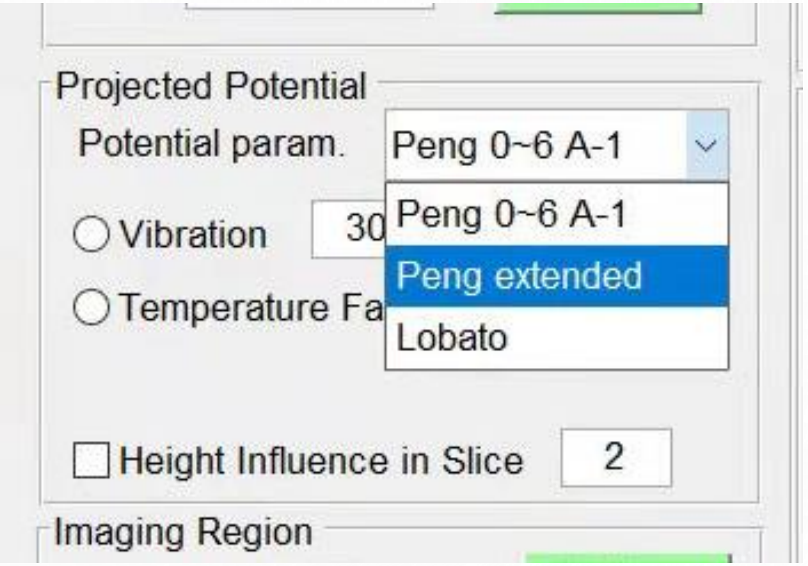


$$B = \frac{8}{3}\pi^2 < dr^2 > \tag{i}$$

$$V(\vec{r}) = \begin{cases} \int f(\vec{s}) \exp(-Bs^2) \exp(4\pi i \vec{s} \cdot \vec{r})\, d^3 s & \text{(iia)} \\ \int f(\vec{s}) \exp(4\pi i \vec{s} \cdot d\vec{r})\ \exp(4\pi i \vec{s} \cdot \vec{r})\, d^3 s & \text{(iib)} \end{cases}$$

$f(\vec{s})$ is the parameterized scattering factor ignoring the TDS effect

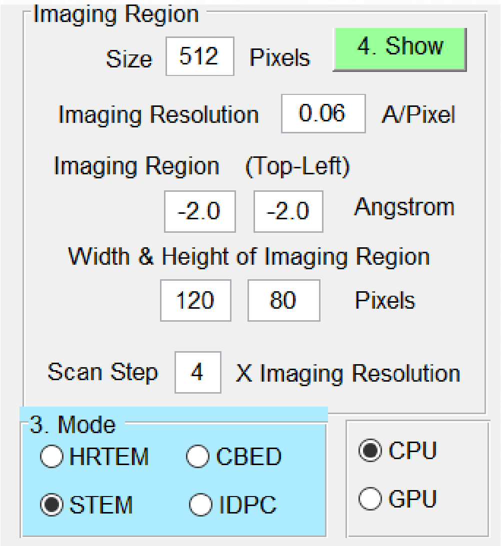
- **Vibration**: All atoms will vibrate according to the DW factor (Eq. i) and input vibration times in the frozen lattice mode. That is, use Eq. iib to simulate TDS.
- **Temperature Factor and Frozen Lattice mode**: use Eq. iia.
- **Height Influence in Slice**: Potential of each atom will contribute to multiple slices and μ value.

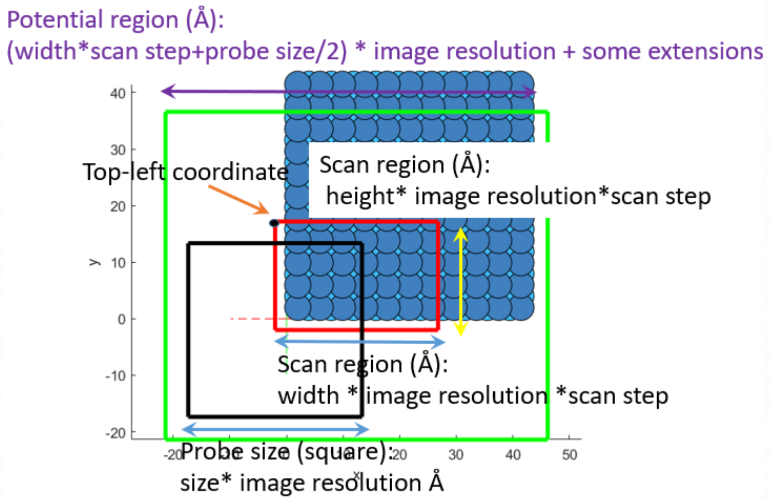


Peng model and Peng extended model can take ‘Height Influence in Slice’, but the potential cannot be assigned in 3D domain if using Lobato model.

3.2 Imaging region

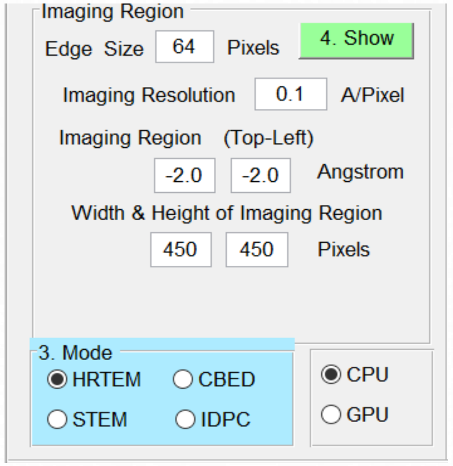
STEM/IDPC Model

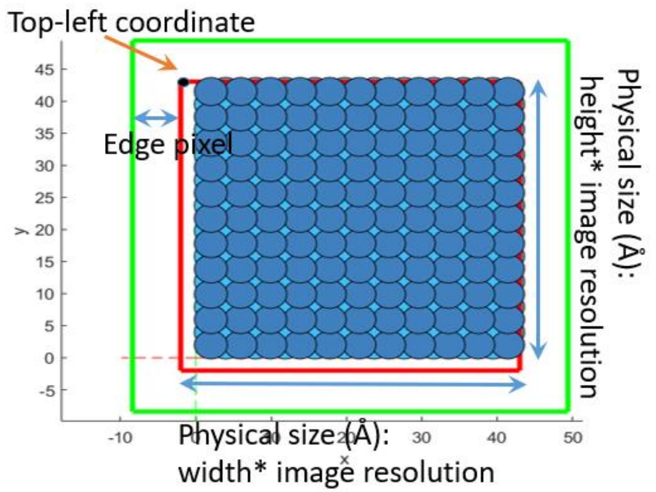




- ➢ Green box: region of the calculated potential, determined by the red and black regions
- ➢ Black box: probe wave's size is in 'Edge Size' and its physical size should be multiplied by 'Imaging Resolution'..
- ➢ 'Imaging resolution': the sampling rate of the probe wave.
- ➢ Red box: the imaging region by editing 'Imaging Region (Top-Left)' and 'Width & Height of imaging Region'.
- ➢ Scan Step: it multiplied by the sampling rate is the sampling rate in the red region.

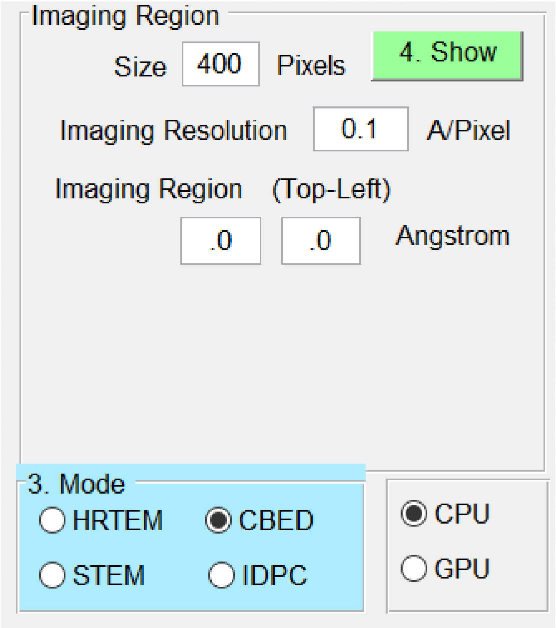
HRTEM Model

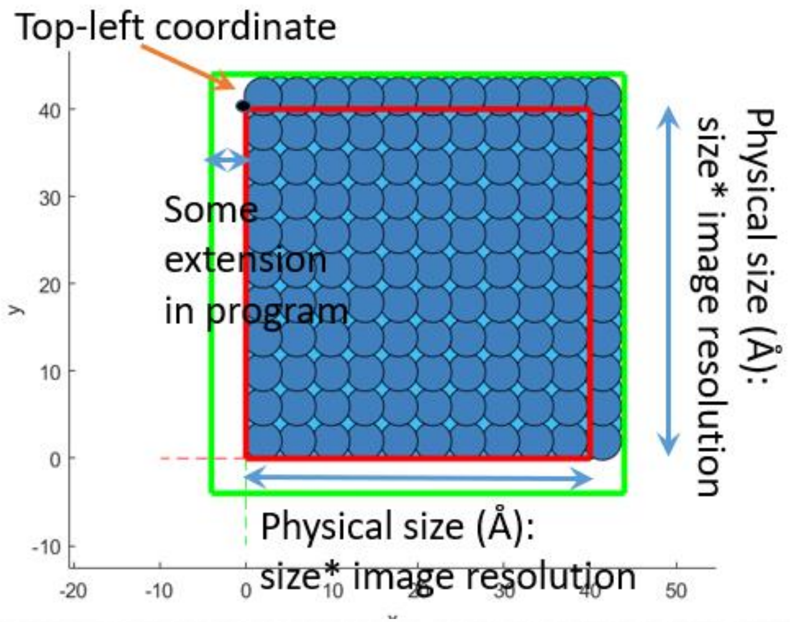




- Green box: region of the calculated potential, determined by the red region and its edge, e.g. the side length is (512+64*2)
- ‘Imaging resolution’: the sampling rate of the image.
- Red box: the imaging region by editing Imaging Region (Top-Left) and Width & Height of imaging Region. Its physical size should be multiplied by ‘Imaging Resolution’.

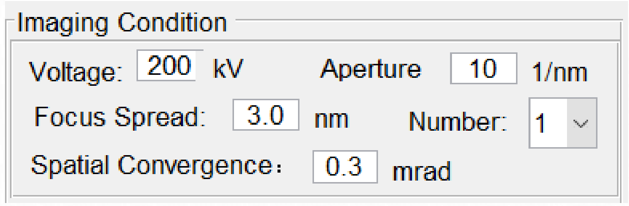
CBED Model





- ➢ Green box: region of the calculated potential, and it is extended by a constant (4 Angstrom) to eliminate the aliasing.
- ➢ Red box: the imaging region by editing Imaging Region (Top-Left) and Width & Height of imaging Region. Its physical size should be multiplied by ‘Imaging Resolution’.

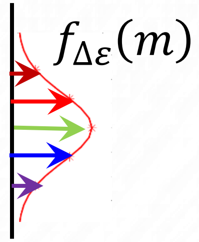
3.3 Coherence



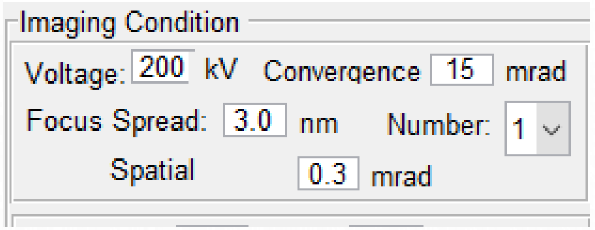
HRTEM Model

- **Voltage**: Accelerated voltage
- **Temporal coherence**: represented by the root mean square of focal spread $\Delta\varepsilon$ (‘Focus Spread’)
- **Spatial coherence**: represented by the semi-convergence angle α of the incident electron beam (‘Spatial Convergence’)
- **Aperture**: Aperture of the objective lens

$$f_{\Delta}(m) = \frac{1}{\sqrt{2\pi}\Delta\varepsilon} exp\left[-\frac{(m\delta\varepsilon)^2}{2\Delta\varepsilon^2}\right] \quad m \in [-M', \dots, 0,1, \dots, M']\ with \sum_{m=-M'}^{M'} f_{\Delta}(m) = 1$$



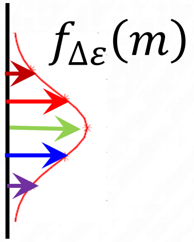
The **2*M+1** is input in ‘Number’ .



STEM/IDPC/CBED Model

- **The temporal coherence**: represented by the root mean square of focal spread $\Delta\varepsilon$ ('Focus Spread')
- **The semi-convergent angle**: the semi-convergence angle α of the incident electron beam ('Convergence')
- **Voltage**: Accelerated voltage

$$f_{\Delta}(m) = \frac{1}{\sqrt{2\pi}\Delta\varepsilon} exp\left[-\frac{(m\delta\varepsilon)^2}{2\Delta\varepsilon^2}\right] \quad m \in [-M', \dots, 0,1, \dots, M']\ with \sum_{m=-M'}^{M'} f_{\Delta}(m) = 1$$



The **2****M*+*1* is input in 'Number' .

3.4 Lens parameters

$\xi = A_\xi \exp(-i\theta_\xi)$

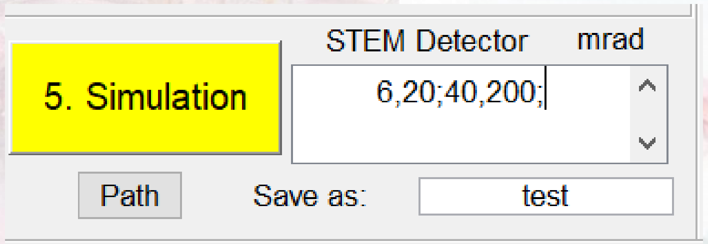
where ξ represents any quantity of astigmatism,
and the wave aberration function χ of lens is written as:

$$\chi(k, \Delta f, A_1, A_2, B_2, \dots) = Re\left\{\frac{1}{2}\Delta f \lambda k k^* + \frac{1}{2}A_1 \lambda k^{*2} + \frac{1}{3}A_2 k^2 k^{*3} + B_2 \lambda^2 k^2 k^* + \frac{1}{4}\mathrm{Cs}\lambda^3 (kk^*)^2 + \frac{1}{4}A_3 \lambda^3 k^{*4} + S_3 \lambda^3 k^3 k^* + \frac{1}{5}A_4 \lambda^4 k^{*5} + D_4 \lambda^4 k^4 k^* + B_4 \lambda^4 k^3 k^{*2} + \frac{1}{6}\mathrm{C}_5 \lambda^5 (kk^*)^3 + \frac{1}{6}A_5 \lambda^5 k^{*6} + R_5 \lambda^5 k^5 k^* + S_5 \lambda^5 k^4 k^{*2}\right\} = \frac{1}{2}\Delta f \lambda k k^* + \frac{1}{4}\mathrm{Cs}\lambda^3 (kk^*)^2 + \chi'(k, A_1, A_2, B_2, \dots)$$

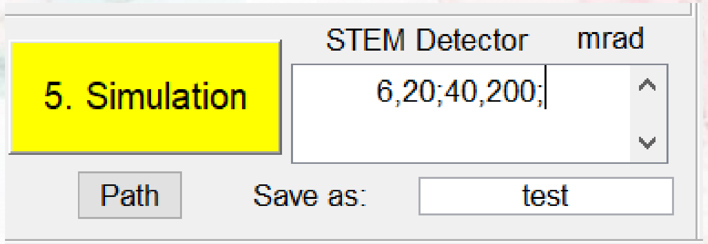
	A_ξ		θ_ξ
Defocus C1:	0	nm	
2-fold astigmatism A1:	0	nm	0
3-fold astigmatism A2:	0	nm	0
Axial coma B2:	0	nm	0
(C3) Cs:	5	um	
4-fold astigmatism A3:	0	um	0
Axial star aberrationS3:	0	um	0
5-fold astigmatism A4:	0	um	0
3-lobe aberration D4:	0	um	0
coma B4:	0	um	0
C5:	0	mm	
6-fold astigmatism A5:	0	mm	0
R5:	0	mm	0
S5:	0	mm	0

3.5 Detectors

➢**STEM modes**: The Angle of the detector is separated by ‘**,**’ , 6 is inner angle and 20 is exterior angle. And different detectors is separated by ‘**;**’.

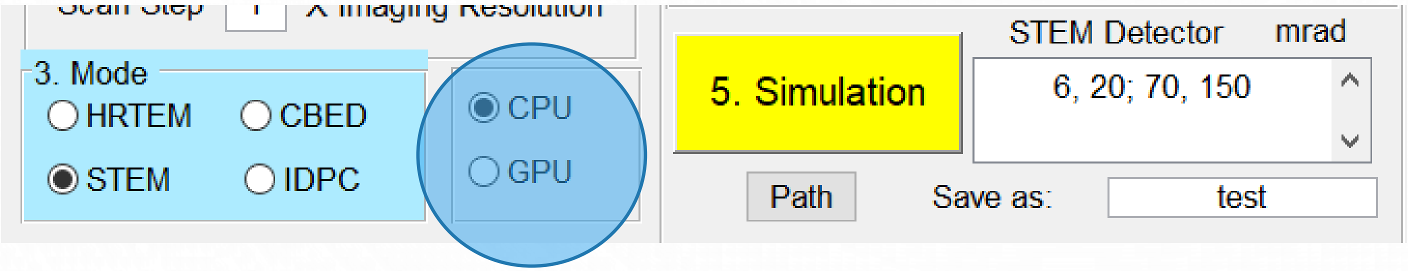


➢**IDPC modes**: The Angle of the detector is separated by ‘**,**’ , 6 is inner angle and 20 is exterior angle. And different detectors is separated by ‘**;**’.

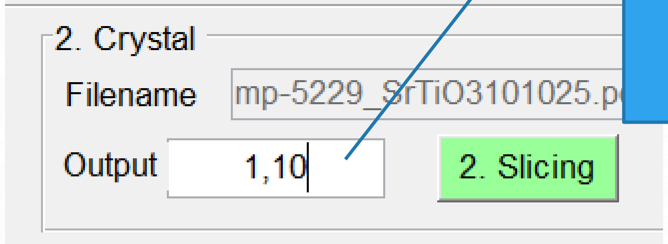


4.Other functions

4.1 STEM/IDPC/CBED related

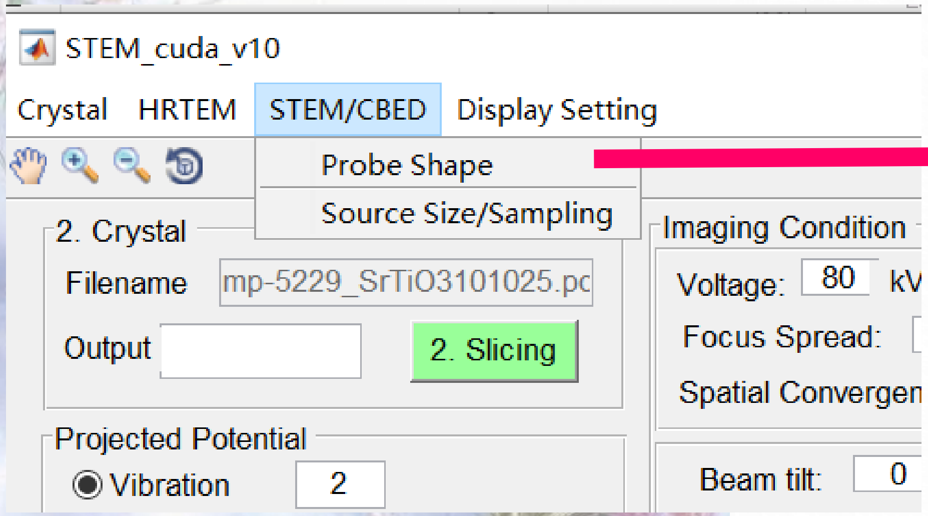


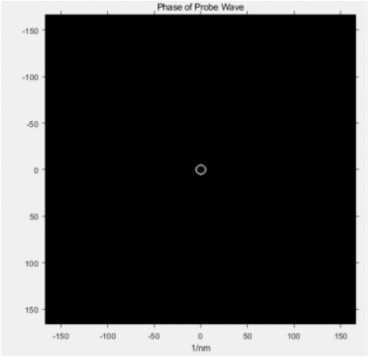
➢ **HRTEM/CBED /STEM/IDPC modes**: users can use GPU/CPU multi-thread parallels.

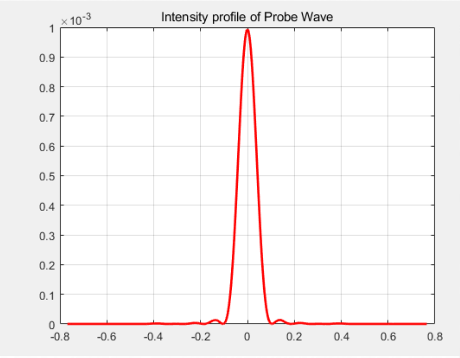


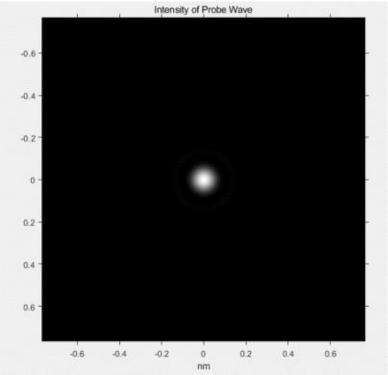
In this input box enter the serial number of intermediate slices you want to output.

Note: The serial number must be an increasing sequence, and numbers are separated by ‘,’ .





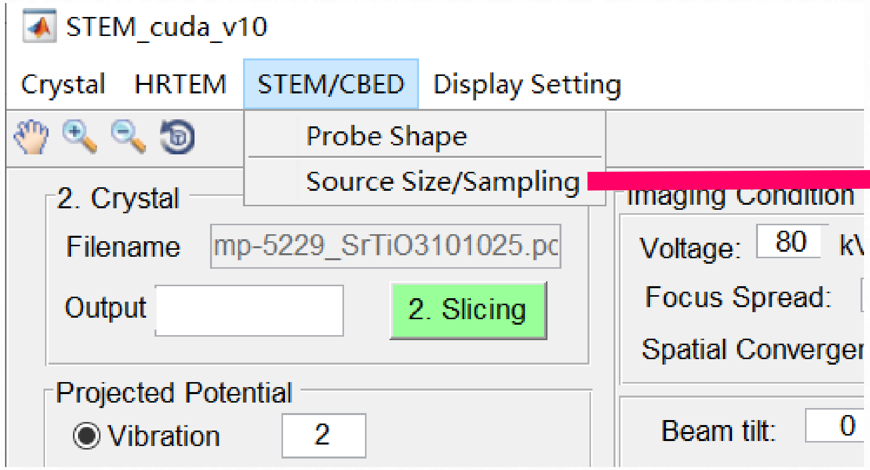


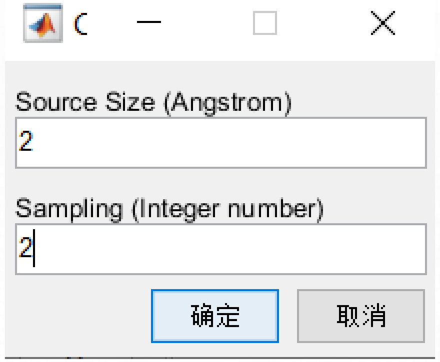


Intensity profile of Probe Wave

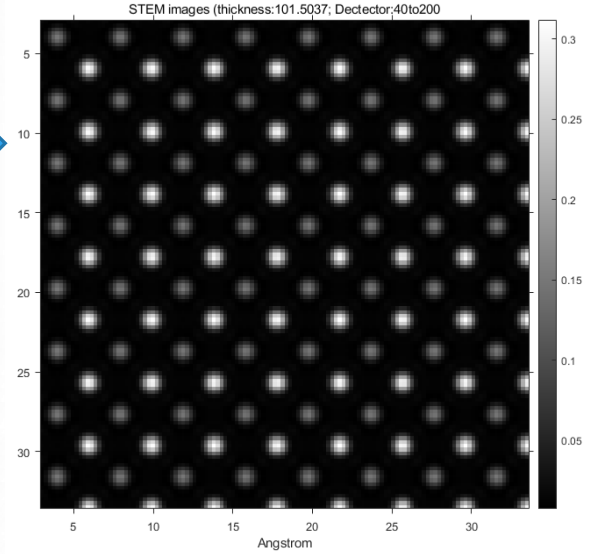
Phase of probe wave

Intensity of probe wave

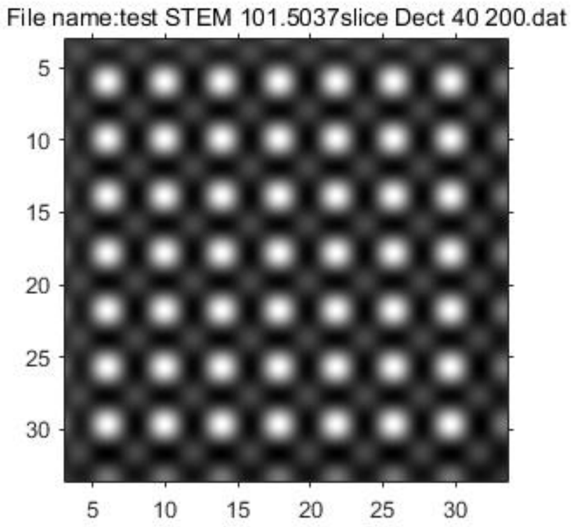




Result

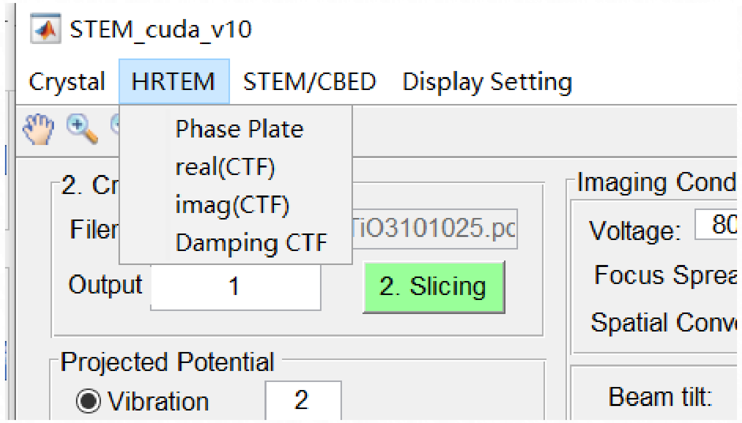


Blurred image

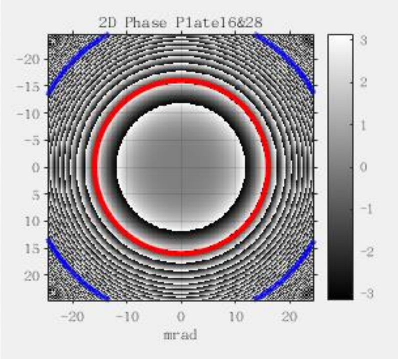


The STEM image can be blurred by a Gaussian function with a specified full width at half maxima (FWHM) and increasing the sampling, which is designed with reference to QSTEM.

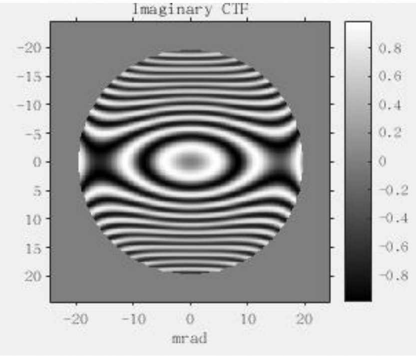
4.2HRTEM related



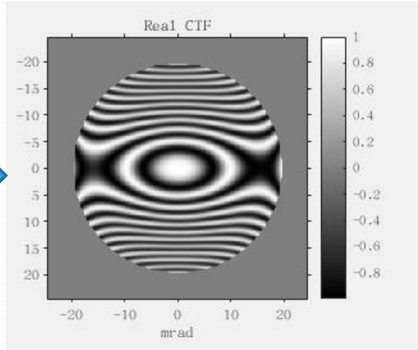
Phase plate



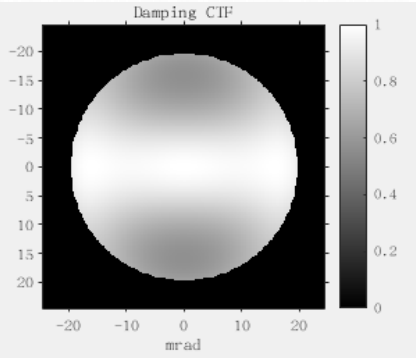
imag(CTF)



Real(CTF)

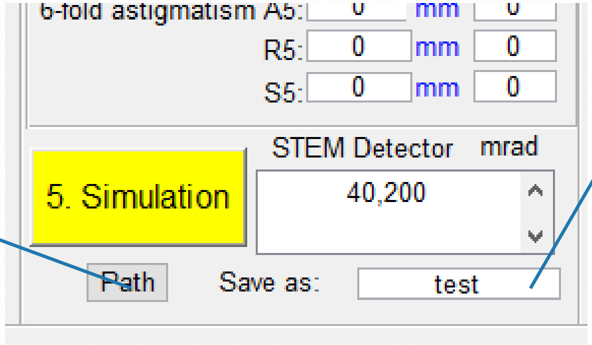


Damping(CTF)



4.3 Save the file

Select the folder to store the results



Name of result

The result will be named as test_STEM_101.5037slice_Dect_40_200.dat

name model thickness Detector angle

If the STEM image is blurred by a Gaussian function, the result will be named as test_STEM_101.5037slice_Dect_40_200_source_2_zoom2.dat

Value of source Value of sampling

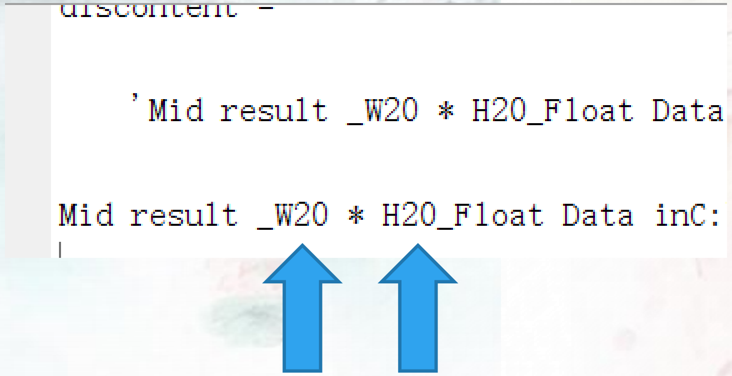
Open the files with the.dat suffix in matlab

fid=fopten(‘file name’, ’r’);

data=fread(fid,[size, size],’float’);

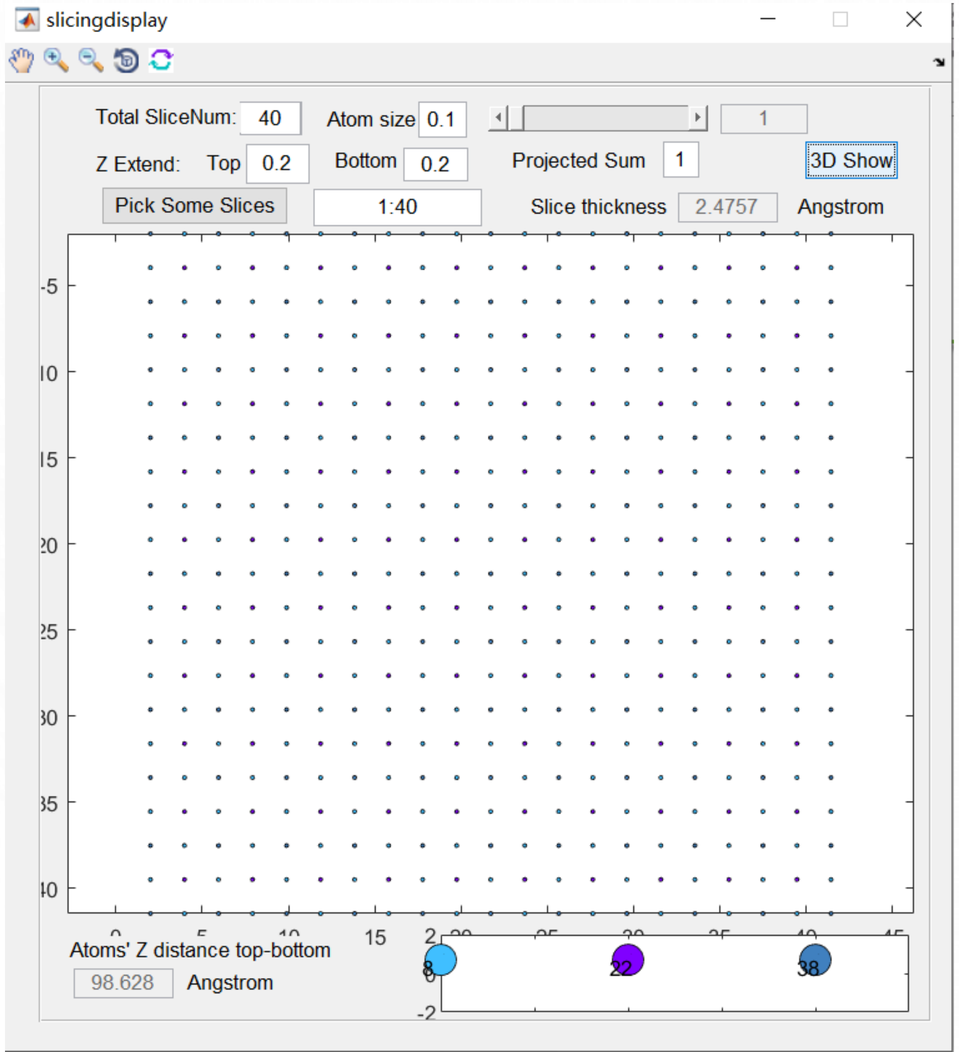
fclose(fid);

data=data’;



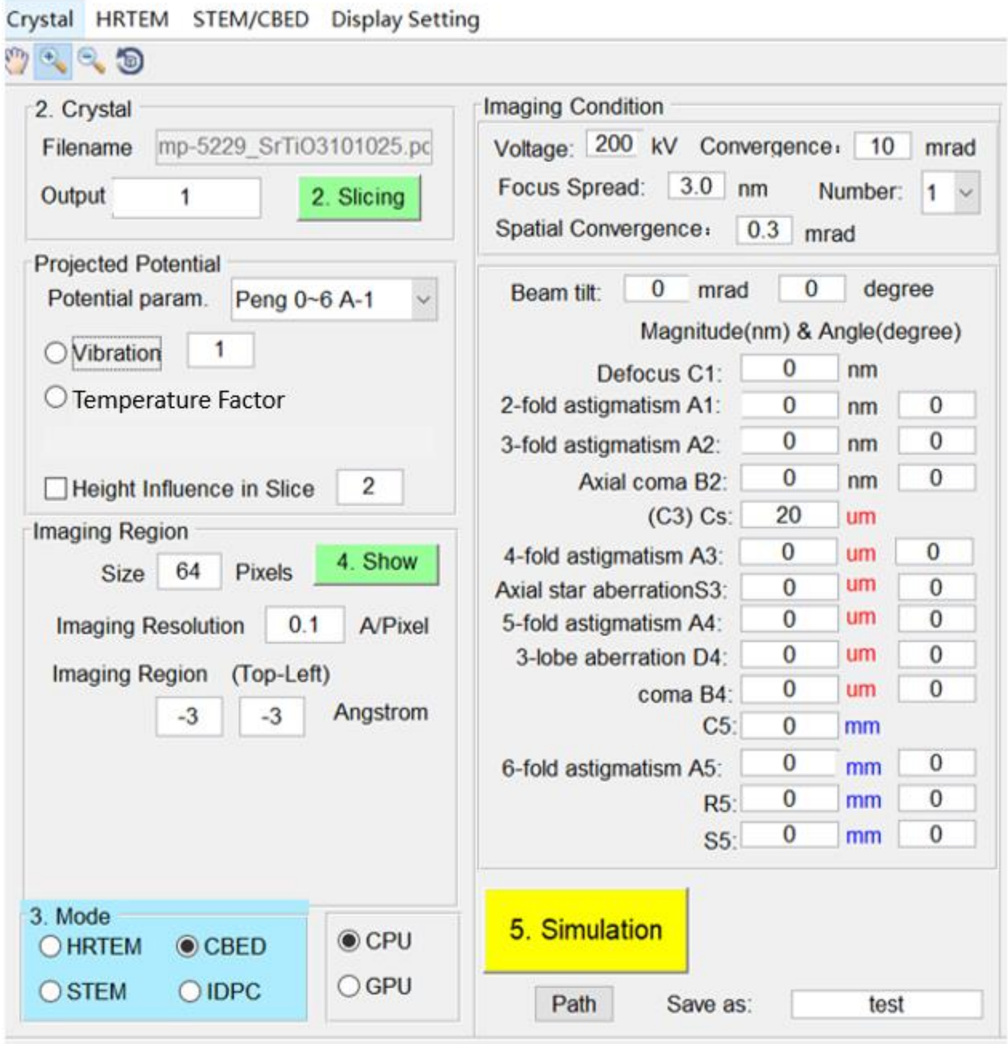
Size: Output at the end of the program

5.Example



The simulation uses the $SrTiO_3$, the pictures is the slicing interface parameter setting, The slicing interface settings of all modes are the same. The interface parameter settings of different modes are different, and they will be given in different modes. The parameters of the potential calculation use Peng's parameters.

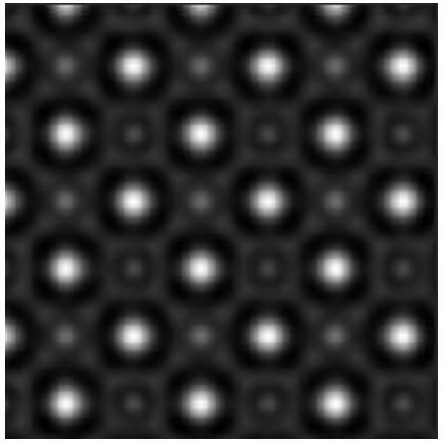
5.1 HRTEM



interface

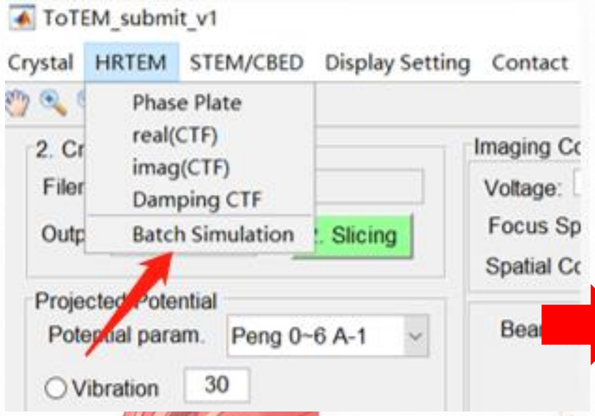
Thickness is 101.5037Å

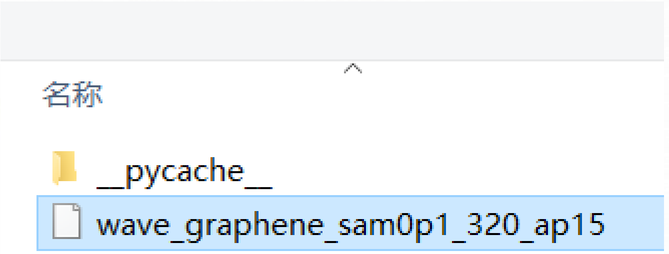
result



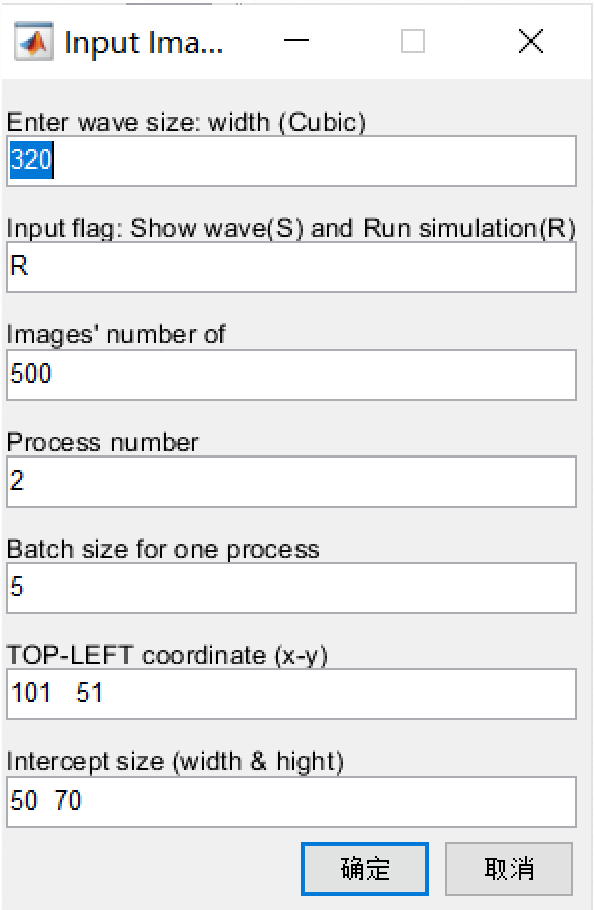
5.1.2 Batch HRTEM Simulation

Application:The simulation image can be produced in large quantities within a certain astigmatic range





Exit wave function
generated in HRTEM mode



Please do not change the format of this file!

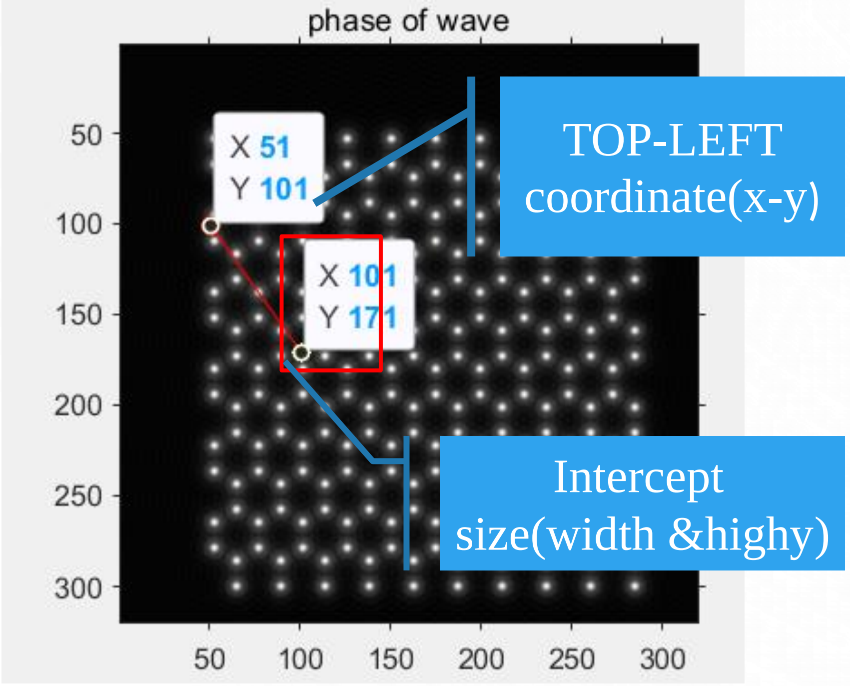
Image's number of: The number of images generated

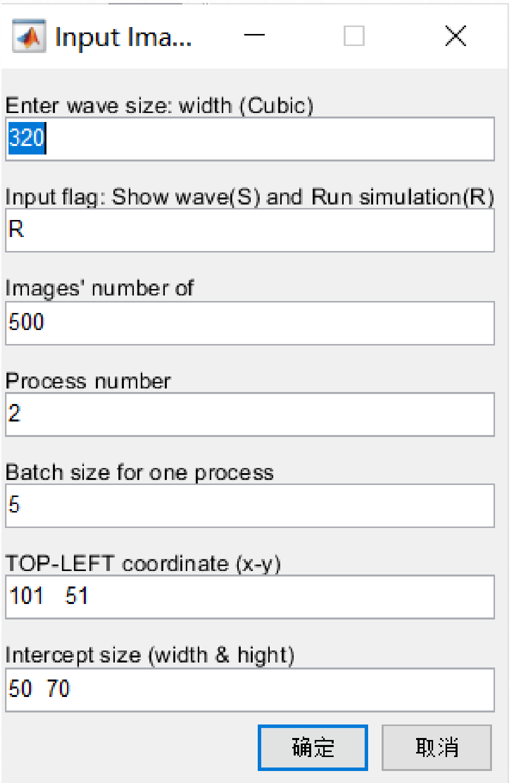
Process number: Number of processes

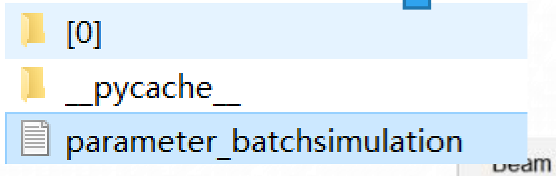
Batch size for one process: The number of images generated per batch per process

Run simulation(R): start to generate images

Show wave(s): display the phase of wave and show the interception area





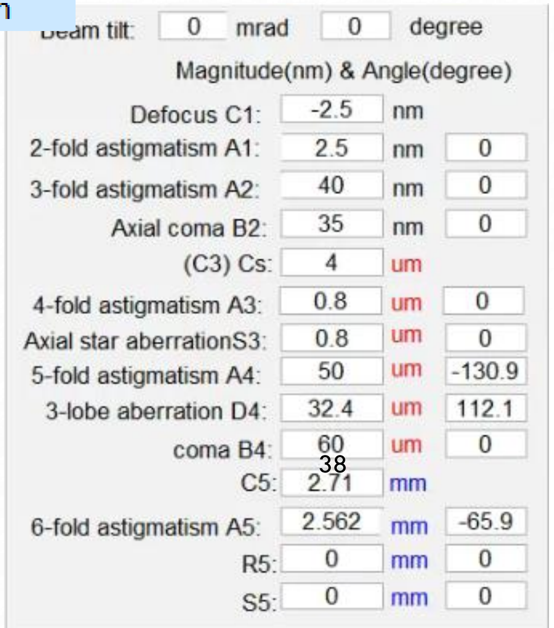



parameter_batchsimulation.txt - 记事本

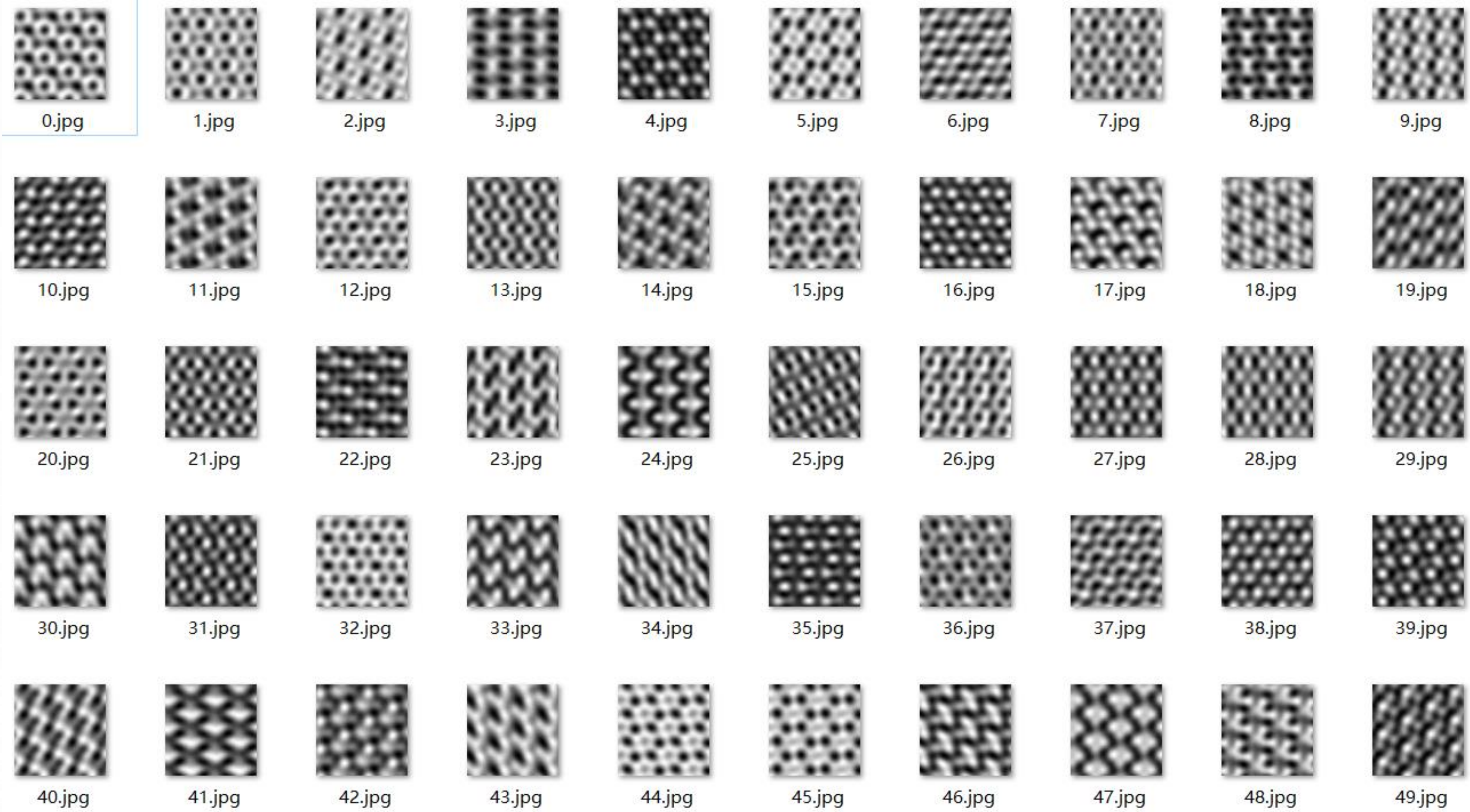
文件(F) 编辑(E) 格式(O) 查看(V) 帮助(H)

```
4     % myrandrange.focus=allvalue(1) %units: nm will be chanced with both positive and nagative directions
2.5   %myrandrange.A1=allvalue(2)       %units:nm
180   %myrandrange.phiA1=allvalue(3);    %units:degrees  max 180
10    %myrandrange.A2=allvalue(4);      %units:nm
180   %myrandrange.phiA2=allvalue(5);  %units:degrees  max 180
10    %myrandrange.B2=allvalue(6);      %units:nm
180   %myrandrange.phiB2=allvalue(7);  %units:degrees  max 180
1000 %myrandrange.Cs=allvalue(8);       %unit nm  ****
700   %myrandrange.A3=allvalue(9);      %units:nm  ****
180   %myrandrange.phiA3=allvalue(10); %units:degrees  max 180
600   %myrandrange.S3=allvalue(11);     %units:nm ****
180   %myrandrange.phiS3=allvalue(12); %units:degrees  max 180
50000 %myrandrange.A4=allvalue(13);    %units:nm ****
180    %myrandrange.phiA4=allvalue(14);%units:degrees  max 180
0  %myrandrange.D4=allvalue(15);         %units:nm ****
0  %myrandrange.phiD4=allvalue(16);      %units:degrees  max 180
0  %myrandrange.B4=allvalue(17);         %units:nm ****
0  %myrandrange.phiB4=allvalue(18);      %units:degrees  max 180
0  %myrandrange.A5=allvalue(19);         %units:nm ****
0  %myrandrange.phiA5=allvalue(20);      %units:degrees  max 180
0  %myrandrange.C5=allvalue(21);         %units:nm ****  %其实也可以设置百分比。
```

Import ranges to randomly generate values around each aberration.

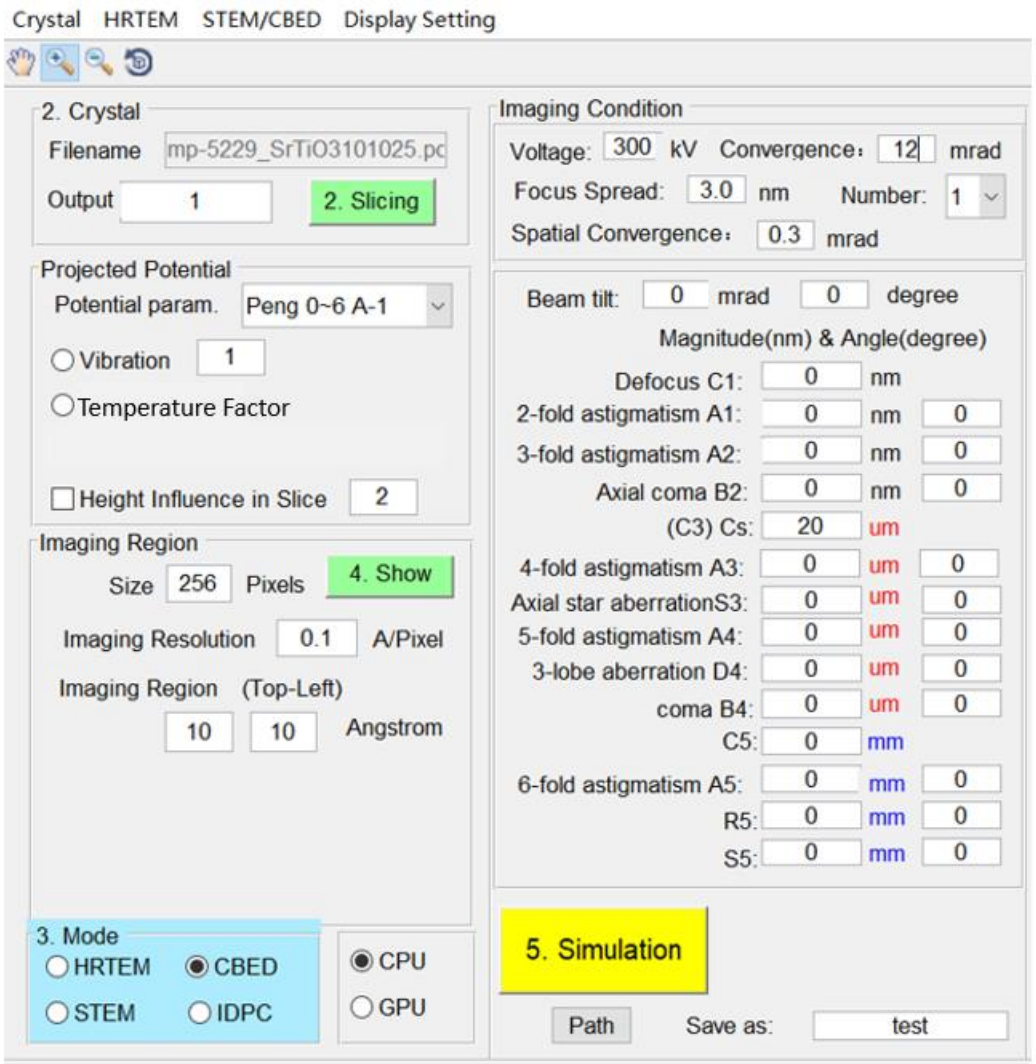


Batch simulation result



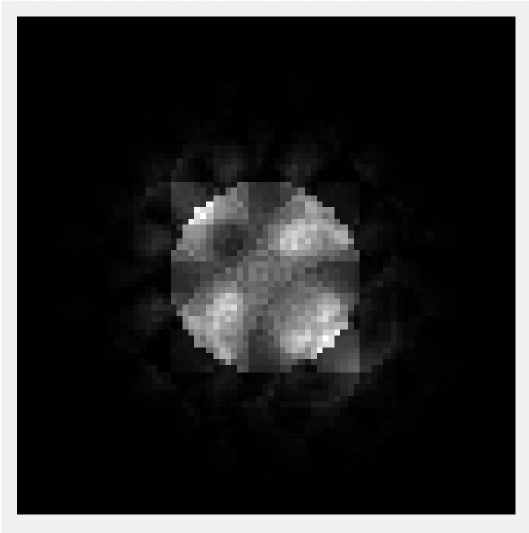
Fifty images of HRTEM model were successfully generated!

5.2 CBED

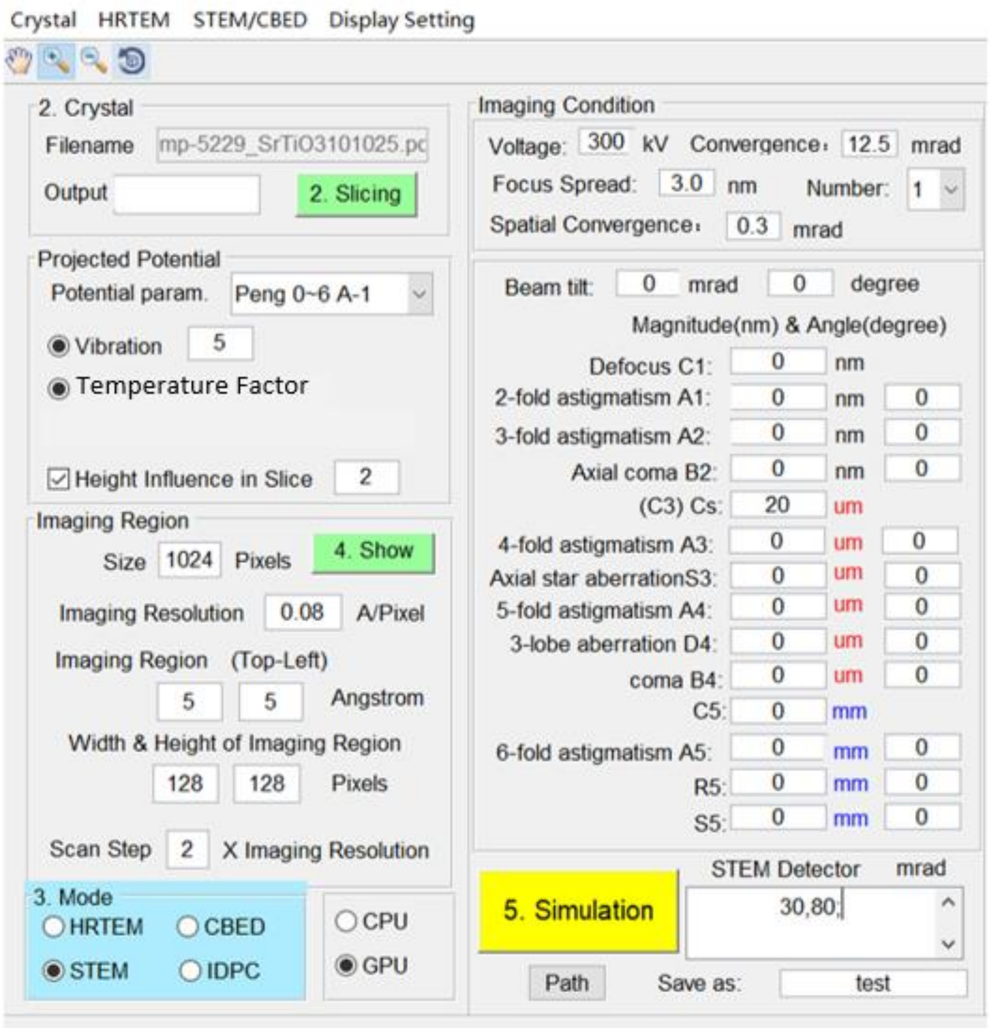


interface

result

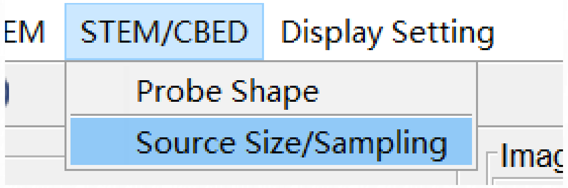


5.3 STEM

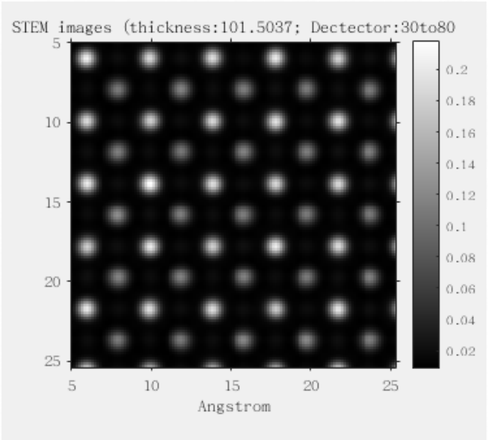


interface

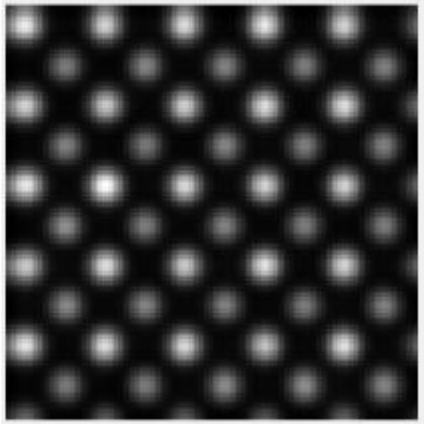
Thickness is 101.5037Å



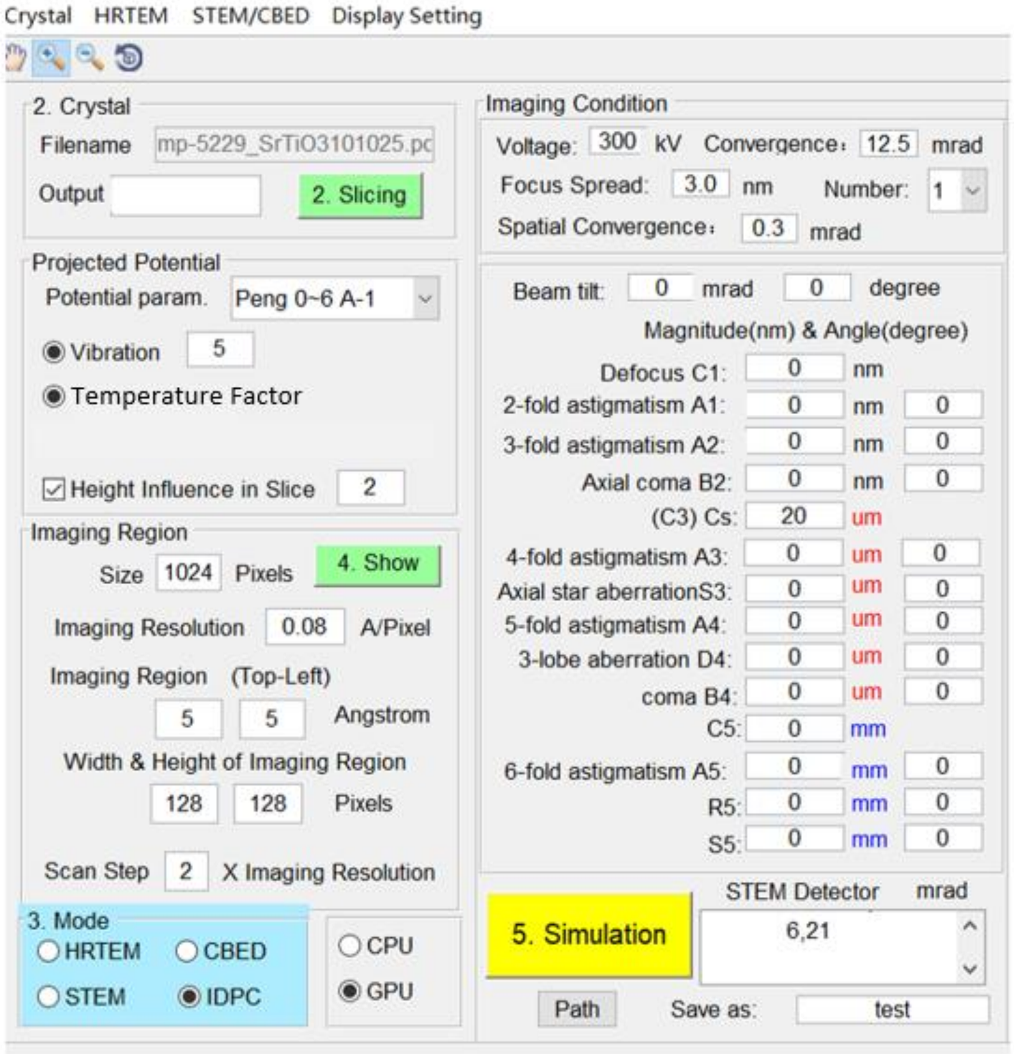
result



blurred by Gaussian Function



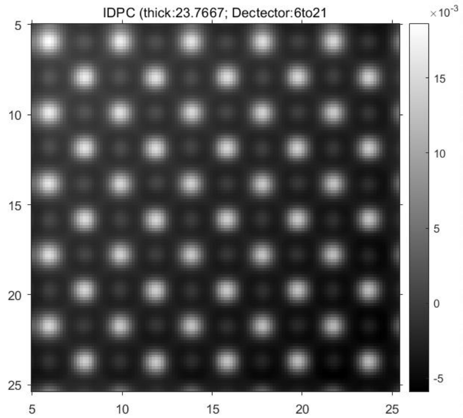
5.4 IDPC



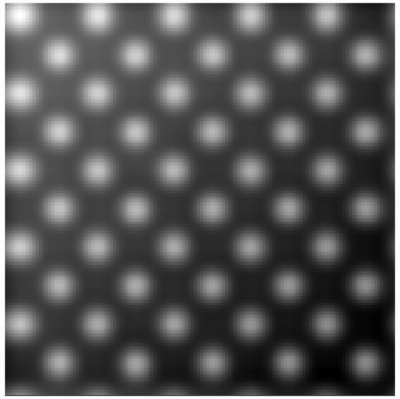
interface

Thickness is 23.7Å

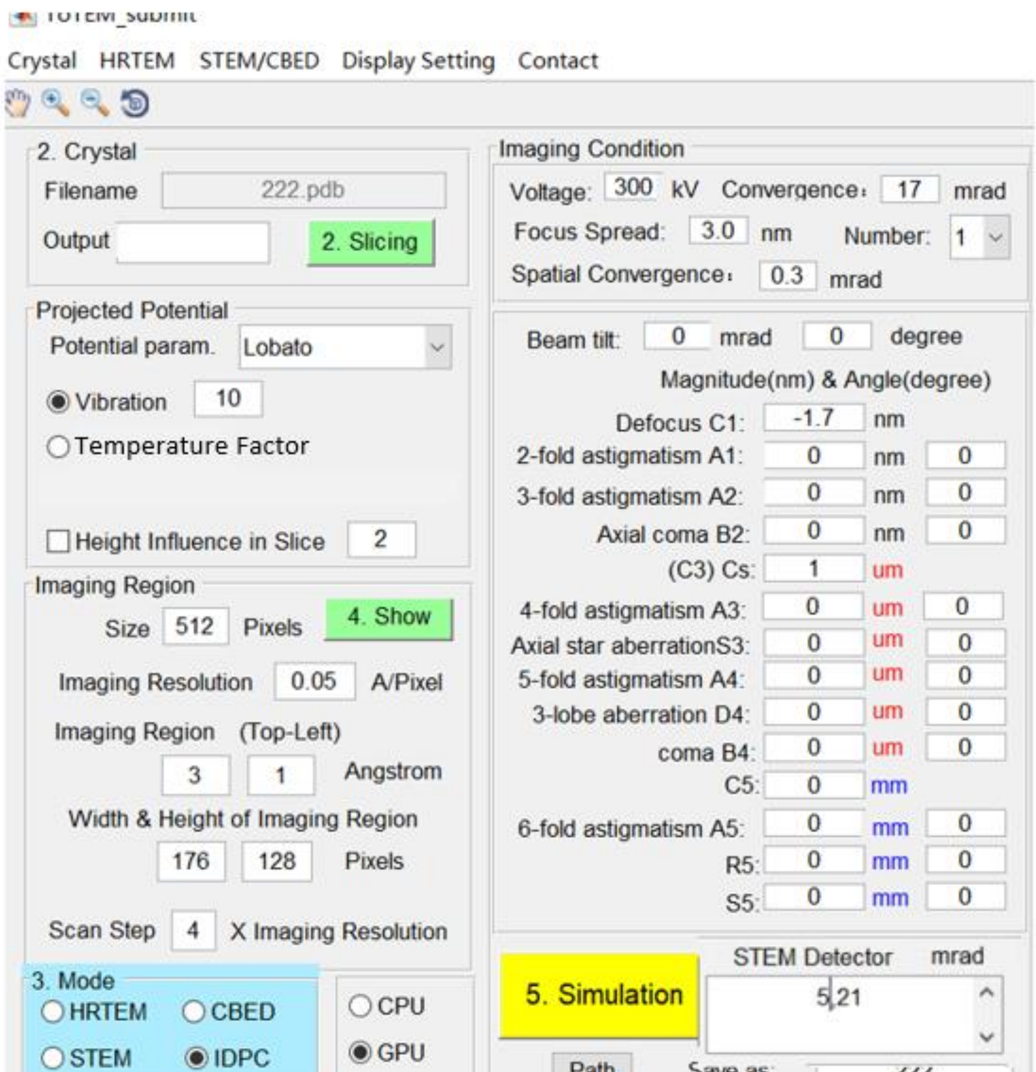
result



blurred by Gaussian Function



5.5 IDPC Simulation for MFI-type zeolites

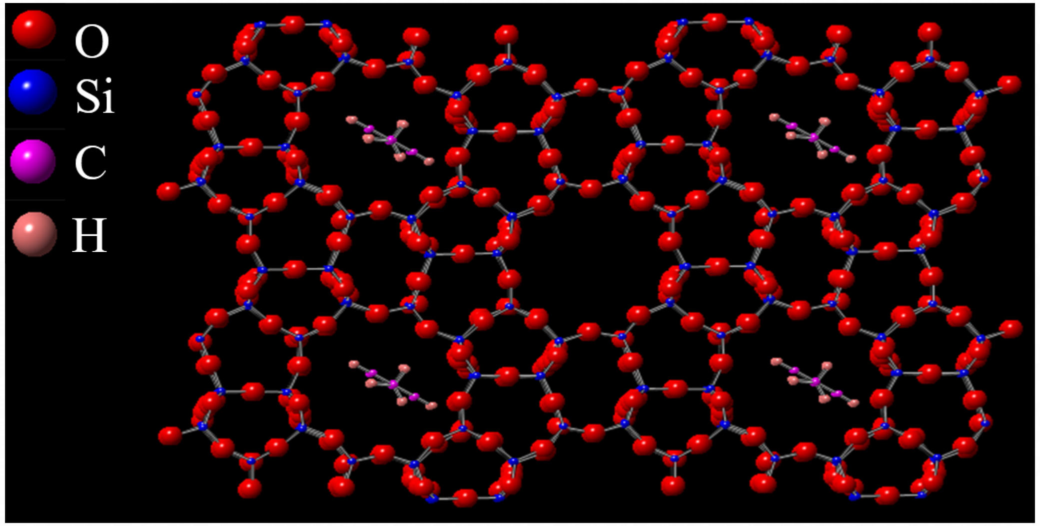


Thickness is 38.3Å

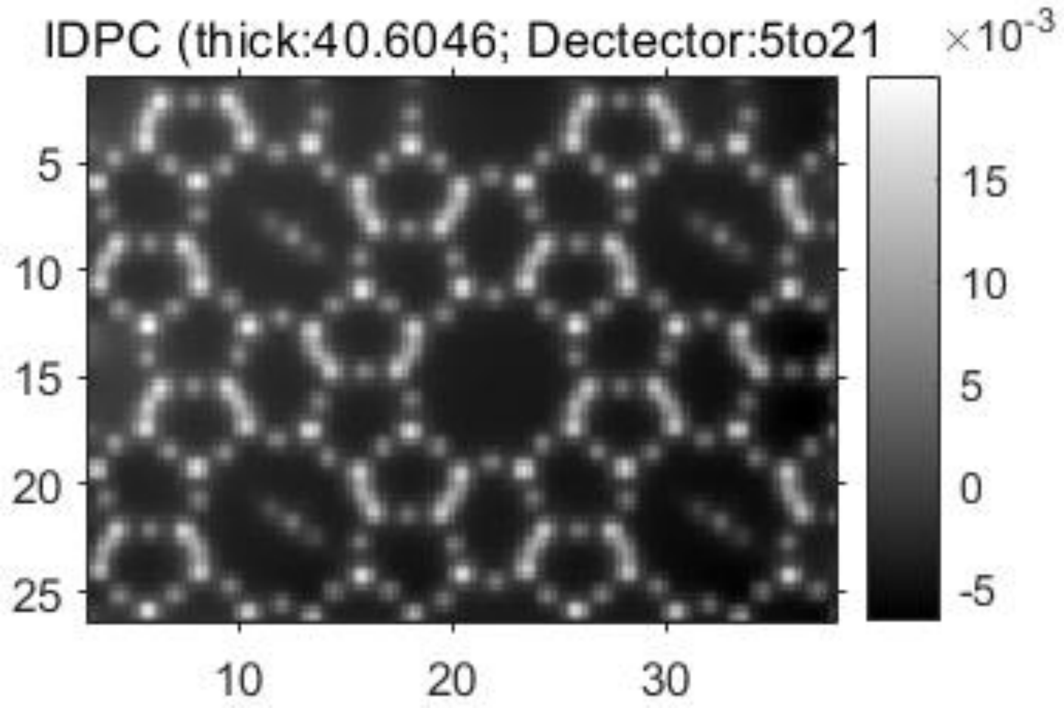
interface

Structure

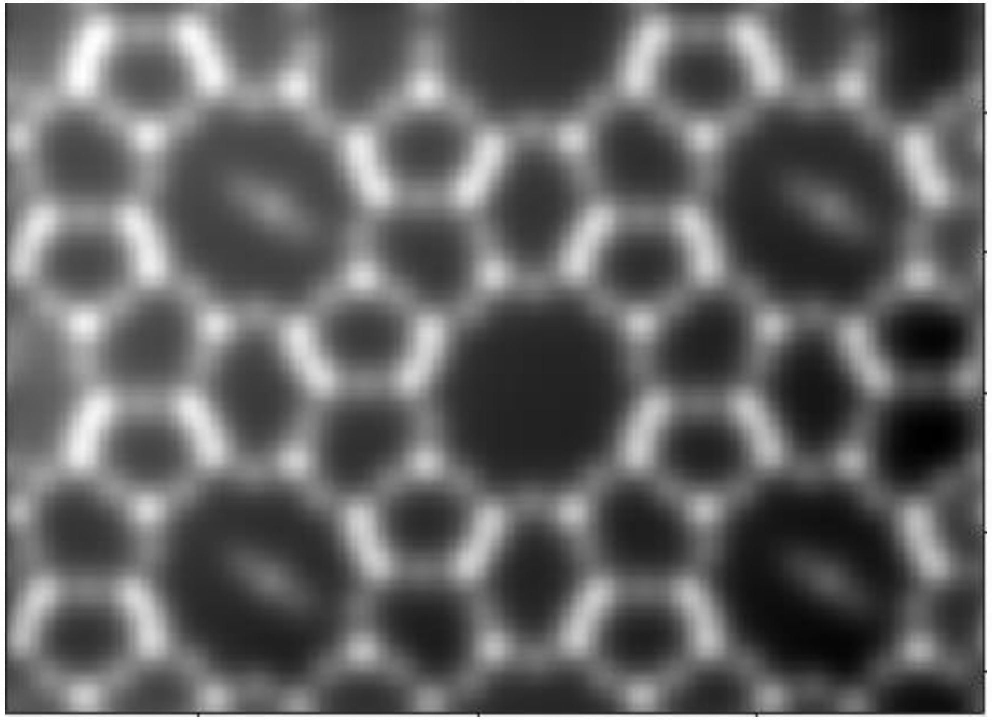
010 direction



result



blurred by Gaussian Function



Prof. Fang Lin developed the codes on CPU and GUI. Mr. PengJun Yuan at Xiangtan University developed the CUDA codes to speed up calculation, and Mr. KePeng Wu tested the program and developed some codes on CPU. Prof. Yuan Yao and Prof. ChuanHong Jin offers theoretical support. Mr. ZhiQun Li at South China University of Technology have done some previous work.

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