Manual of ToTEM Software

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CONTENT

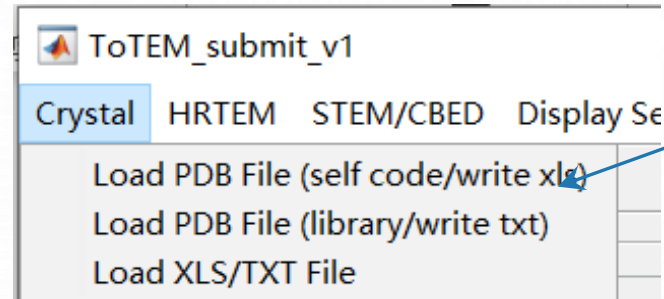- I. QUICK OPERATION.

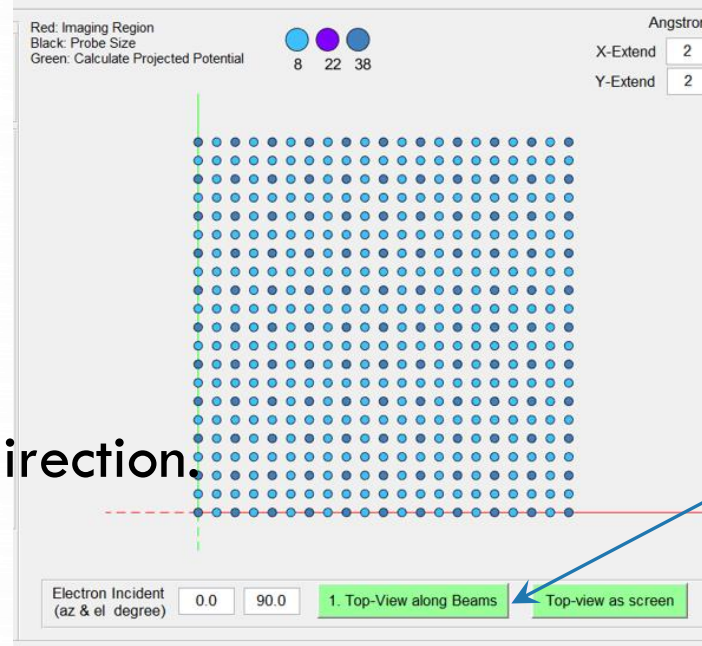- II. ENVIRONMENT CONFIGURATION.

- III. DETAILS

I. QUICK OPERATION

0. <mark>Run mex_cuda.m</mark> and then ToTEM_submit_v1.m (source code).

1、 Read information about a supercell.

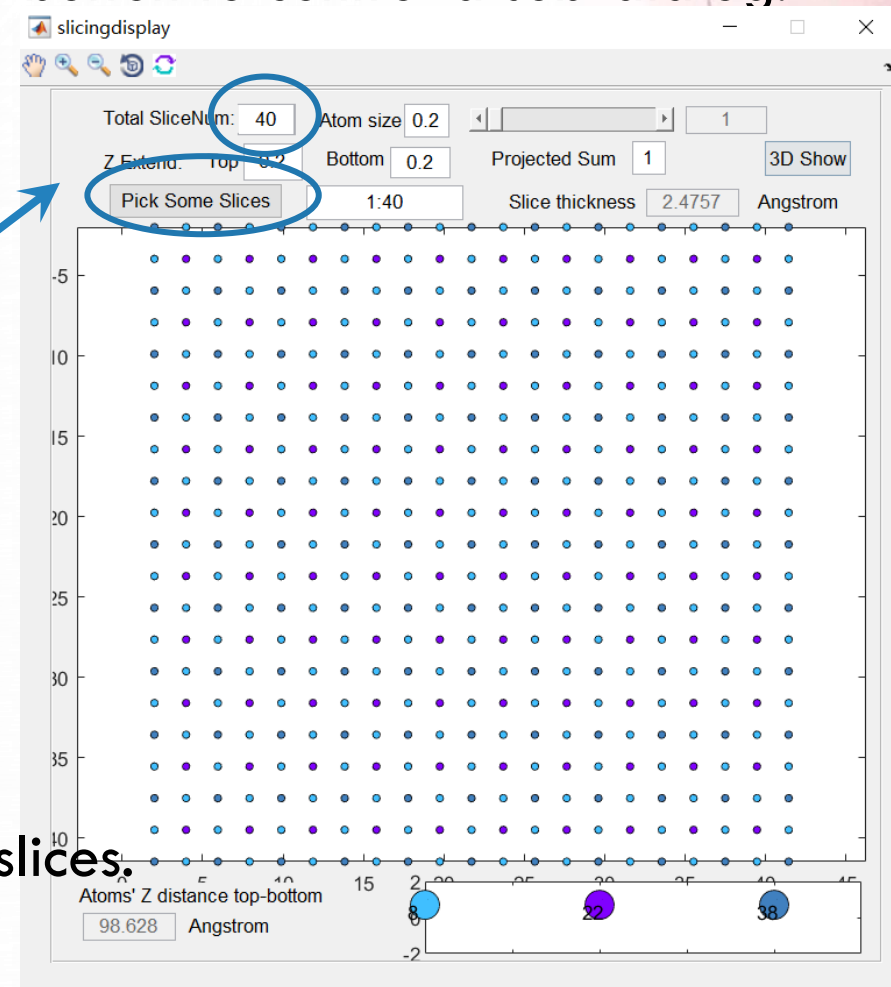2、 Press radio button to get a special direction.

Anyone of three

Anyone of two

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

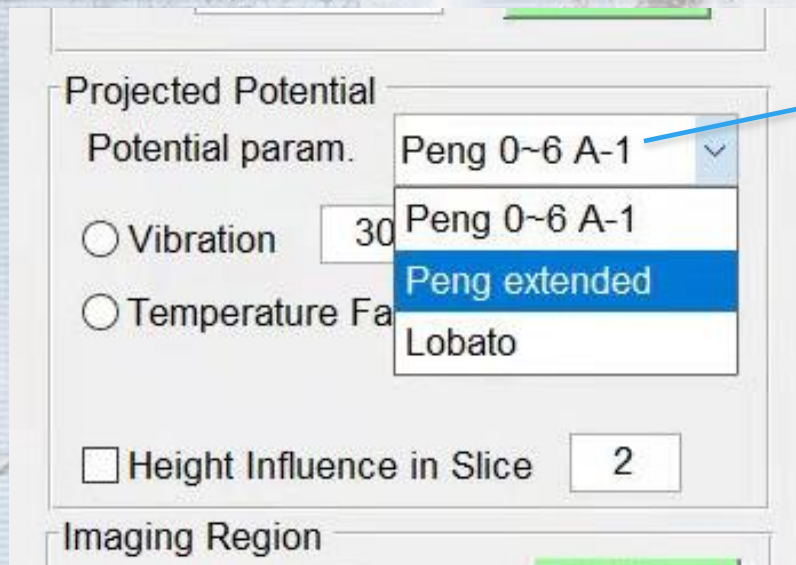3b. Set the total slice number and pick some slices.

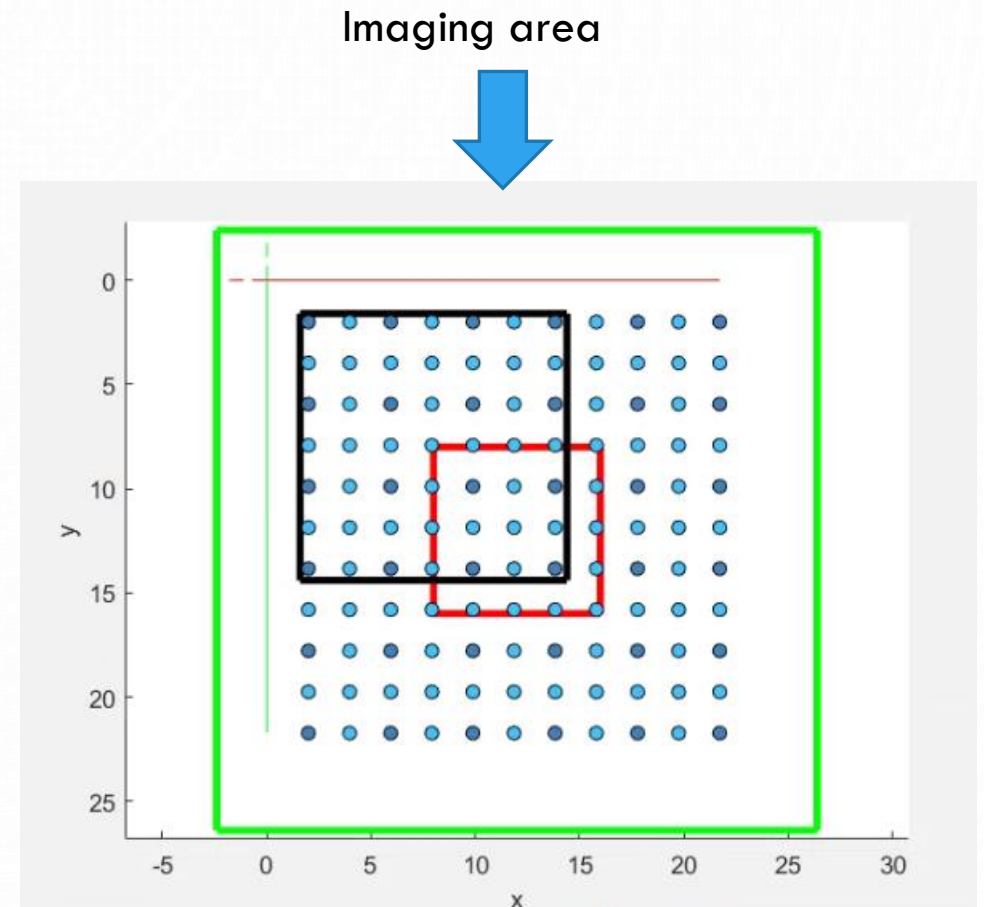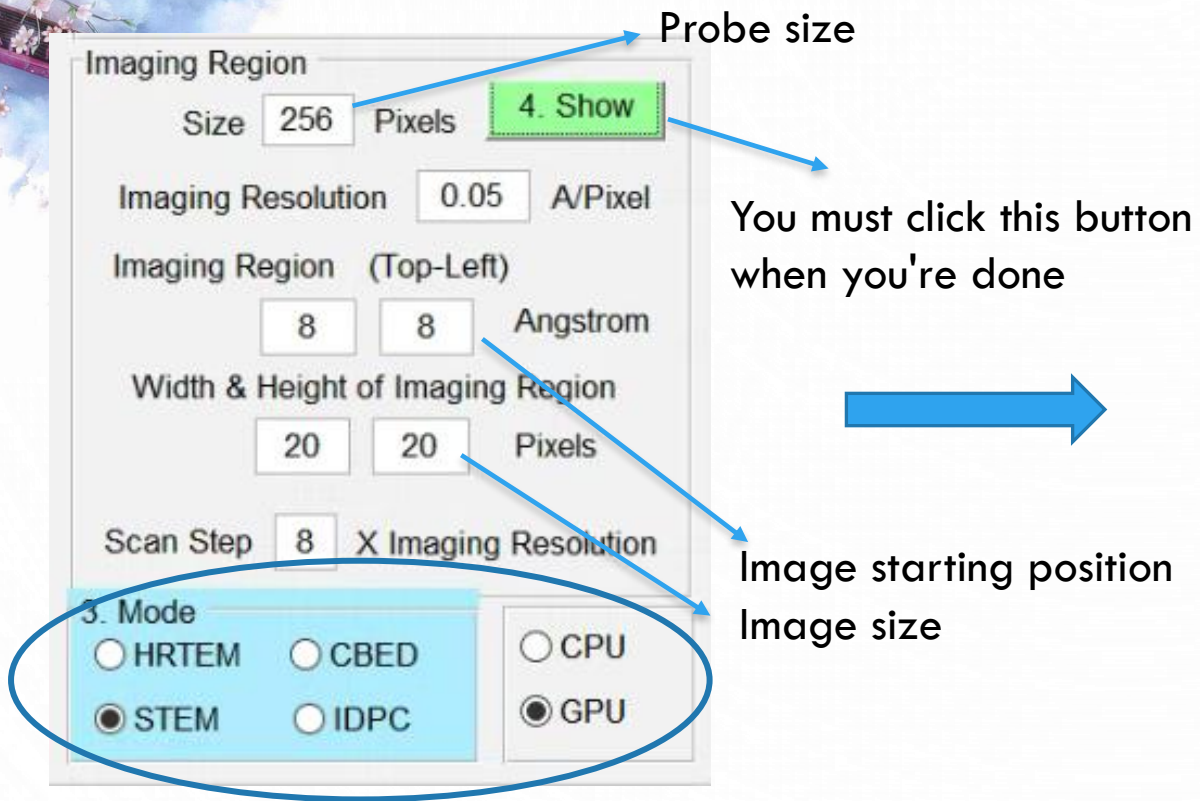4、 Selection for atomic scattering factor and vibration. For example:

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

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.

1 Windows CUDA
Open https://developer.nvidia.com/cuda-downloads to install 'cuda 11 version', then type 'nvcc-v' at the terminal. Installation is successful if display as Fig. 1-1

2 Ubuntu 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.

3 Source codes
Run mex_cuda.m first! And run ToTEM_submit_v1.m. (Note: Run the shell, go to the 'bin' director of Matlab and type 'sh matlab' to run matlab.)
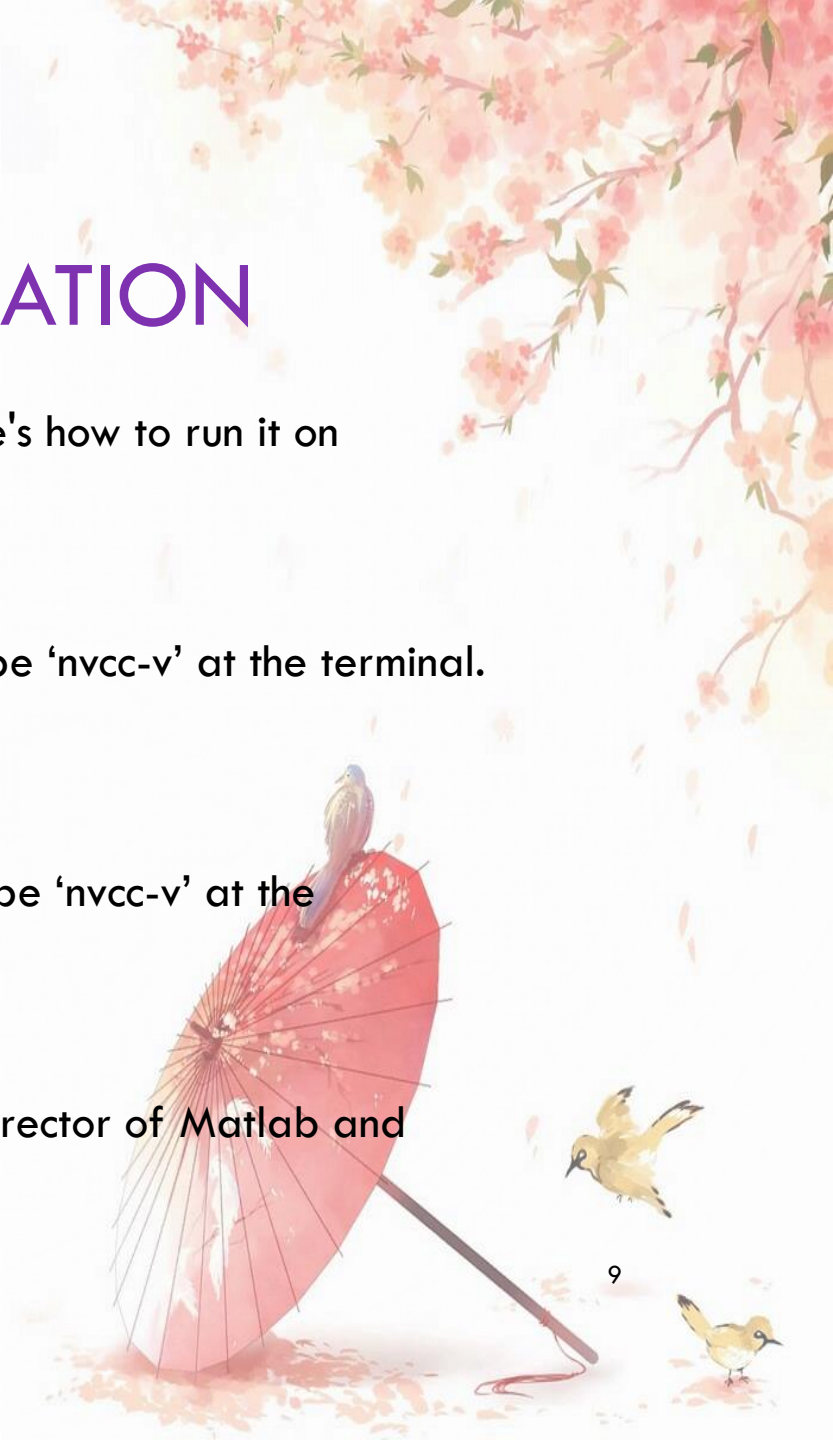
III. DETILS

0. GUI

1. Import a crystal

Import crystal information from a PDB file or an excel or text file.
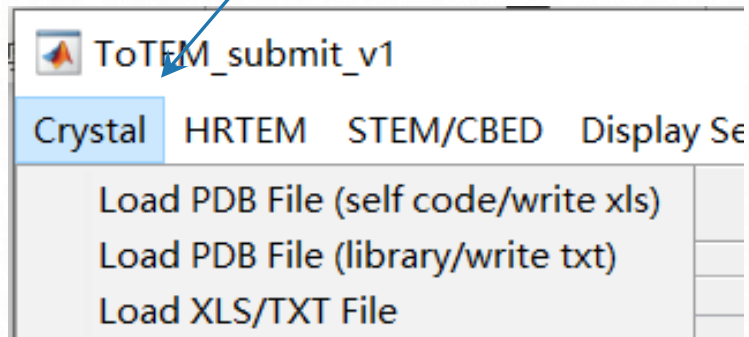
Input Debye-waller (DW) factor for every element. The dialog box will pop up after importing a PDB file

ToTEM_submit_v1

Crystal   HRTEM   STEM/CBED   Display Se

Load PDB File (self code/write xls)
Load PDB File (library/write txt)
Load XLS/TXT File

I.   —   □   ×

DW factor for the 8 Atom

0

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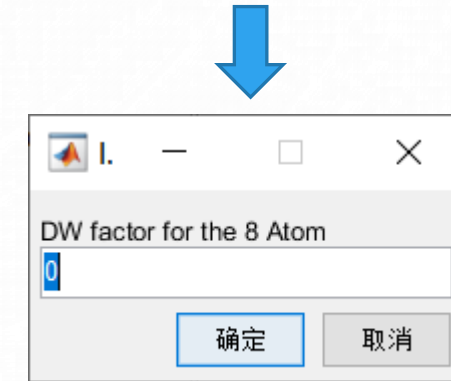
A *.xls or *.txt file will be generated after reading a pdb file.
Next time you can import it without inputting DW factors.

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.

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Red: Imaging Region
Black: Probe Size
Green: Calculate Projected Potential

8 22 38

Angstrom

X-Extend 2

Y-Extend 2

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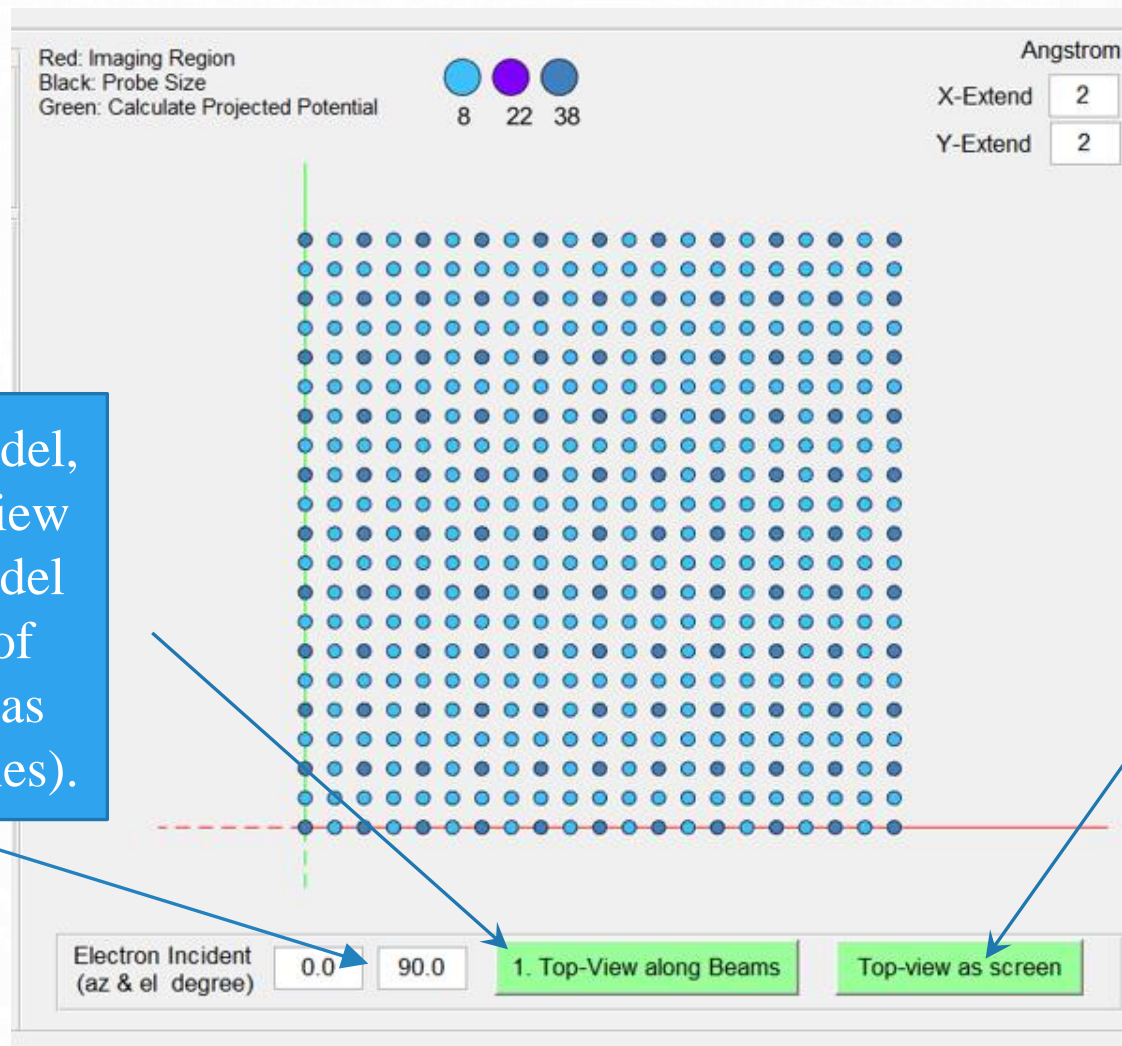
Or you can see the model from any angle after mouse rotating.

Electron Incident
(az & el degree)   0.0   90.0   1. Top-View along Beams   Top-view as screen

Note: at least one button must be clicked

2.Slicing dialog of multislice method

Slider to show any slice.

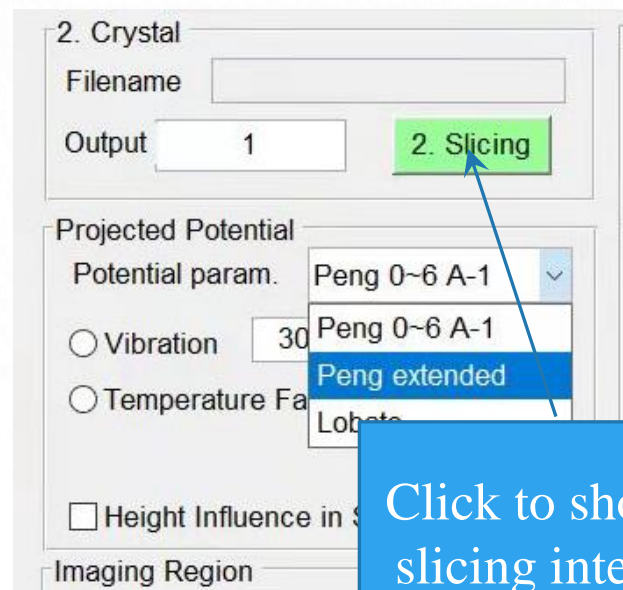After setting the slicing parameters, you must click the button to display the slicing results.
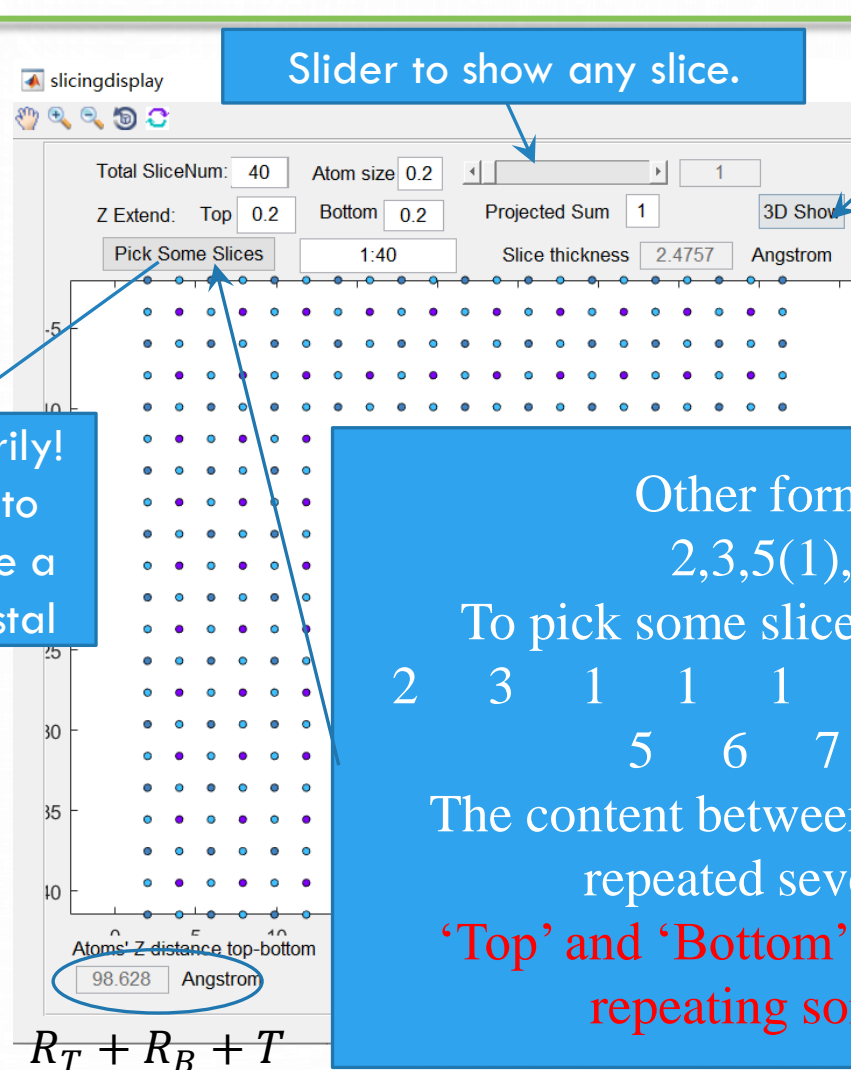
If some atoms were lost after slicing, please add a very small vacuum on top or bottom, such as 0.00001.

slicingdisplay

Total SliceNum:	40	Atom size	0.2		1	3D Show
Z Extend:	Top	0.2	Bottom	0.2	Projected Sum	1
Pick Some Slices		1:40		Slice thickness	2.4757	Angstrom

Atoms' Z distance top-bottom

98.628 Angstrom

$$R_T + R_B + T$$

Necessarily! Click it to generate a new crystal

2. Crystal

Filename

Output 1   2. Slicing

Projected Potential

Potential param. Peng 0~6 A-1

Peng 0~6 A-1

○ Vibration 30 Peng extended

○ Temperature Fa Lobato

□ Height Influence in s

Imaging Region

Click to show the slicing interface.

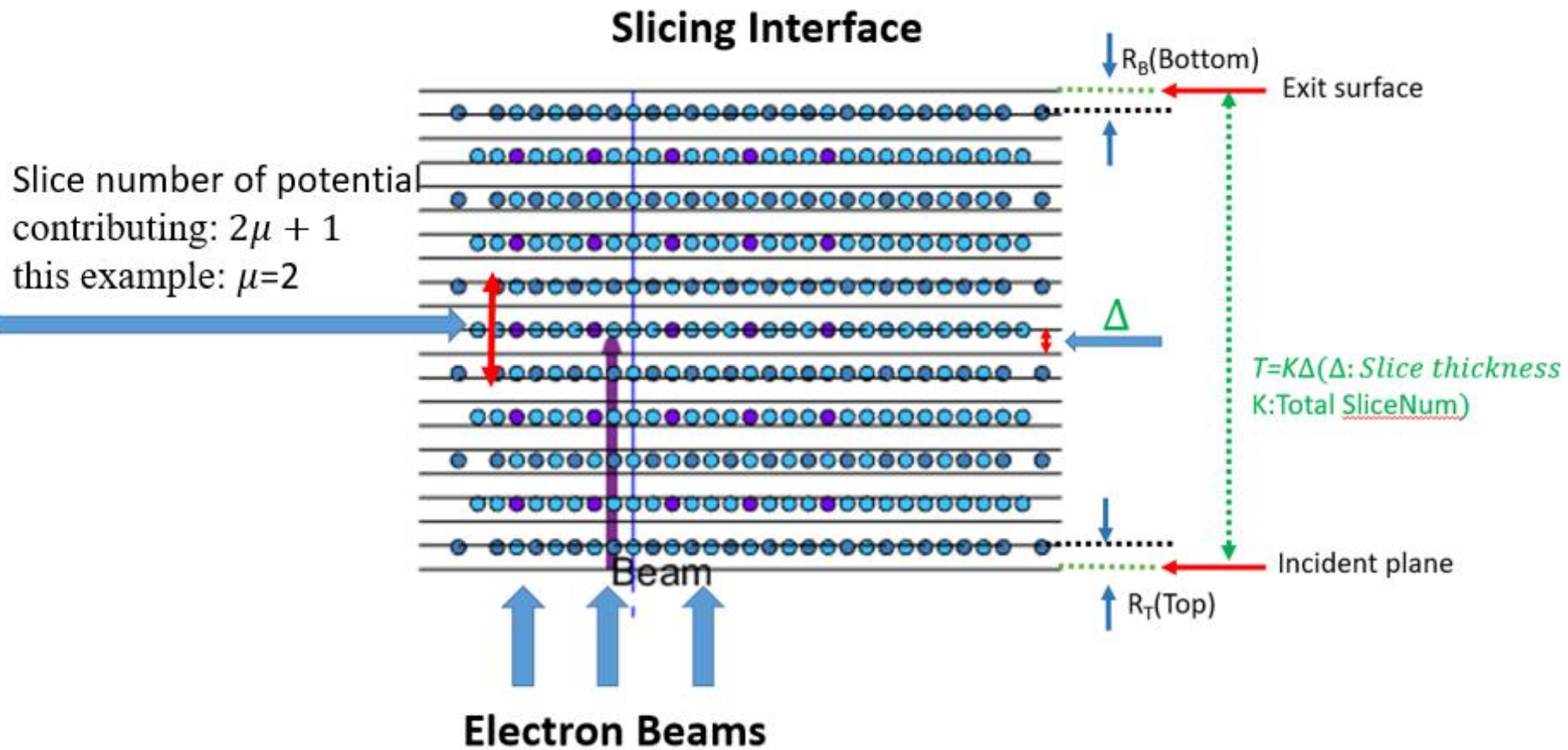Other format like:
2,3,5(1),3(5:7)
To pick some slices from all slices

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

Slicing Interface

Slice number of potential contributing: $2\mu + 1$
this example: $\mu=2$

R_B(Bottom)
Exit surface

Δ

$T=K\Delta$ (Δ: *Slice thickness* K:Total SliceNum)

Incident plane

R_T(Top)

Beam

Electron Beams

3. Parameter settings about simulation

3.1 Vibration, Temperature Factors

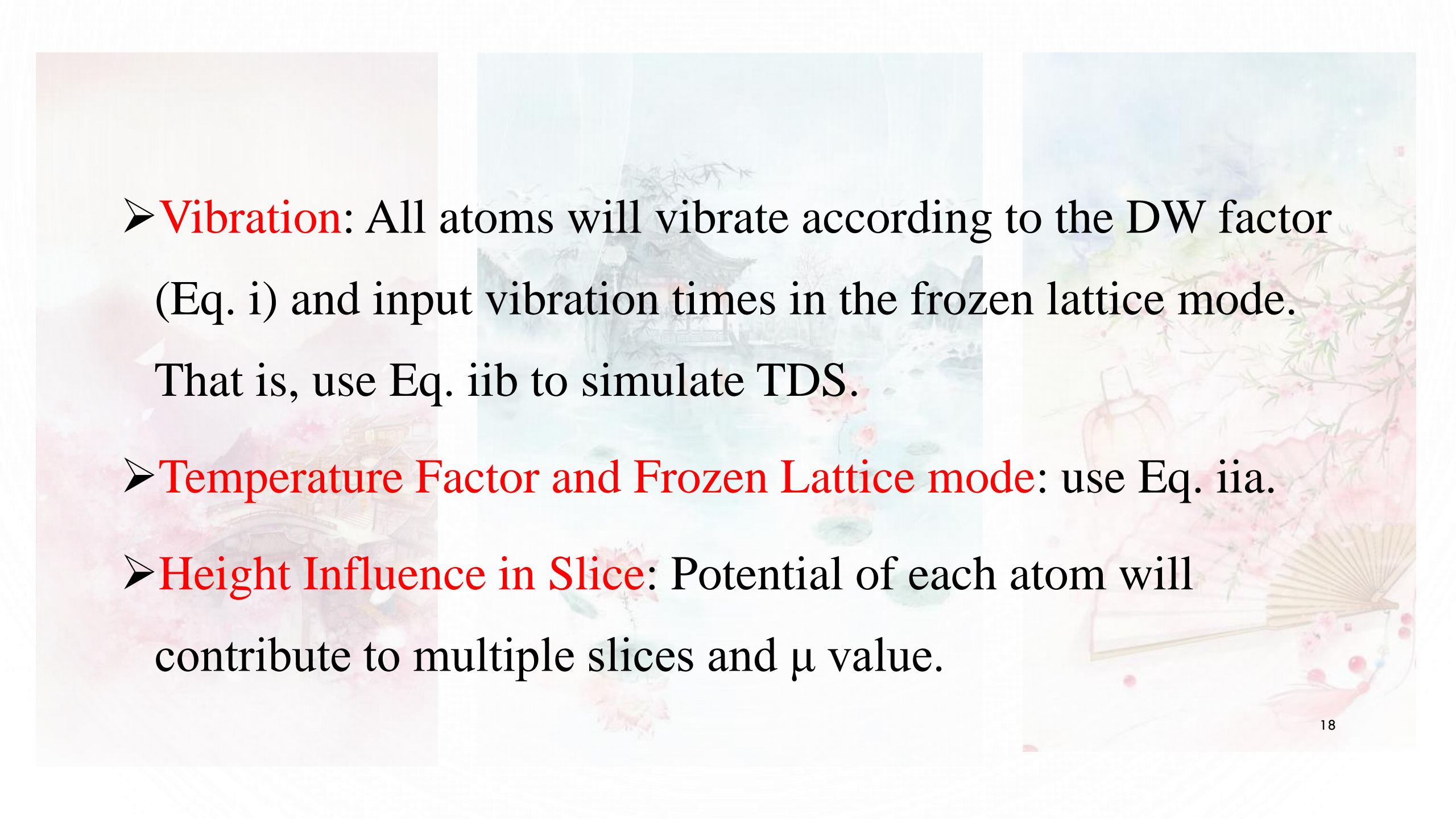

$$B = \frac{8}{3}\pi^2 < dr^2 > \qquad \text{(i)}$$

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

$f(\vec{s})$ is the parameterized scattering factor ignoring the TDS effect
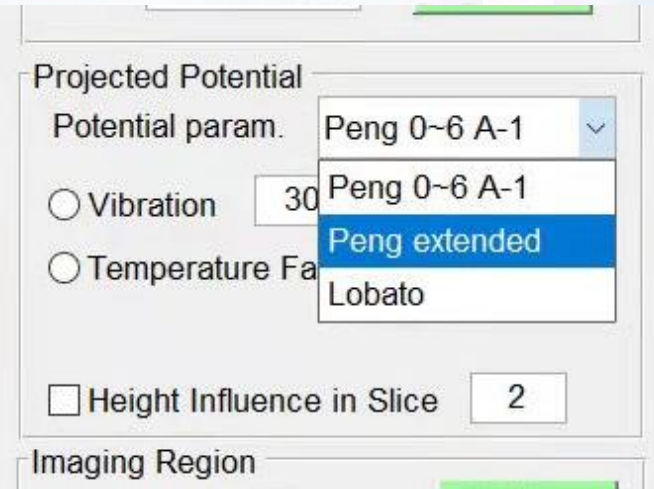
➢Vibration: All atoms will vibrate according to the DW factor (Eq. i) and input vibration times in the frozen lattice mode. That is, use Eq. iib to simulate TDS.

➢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
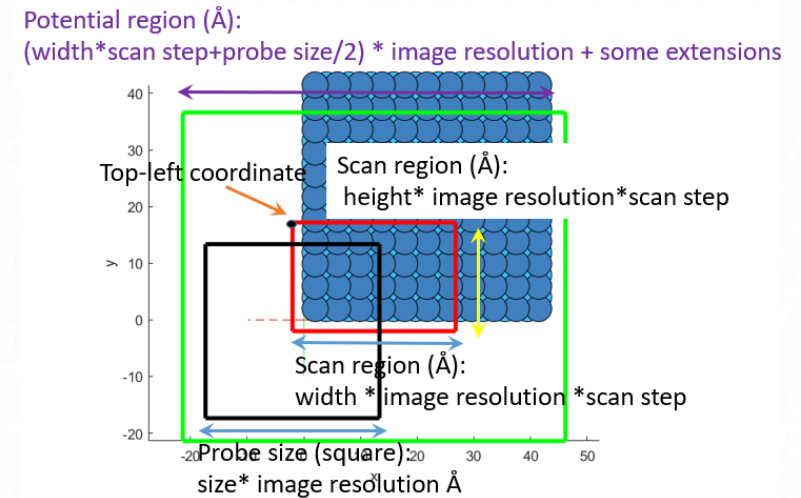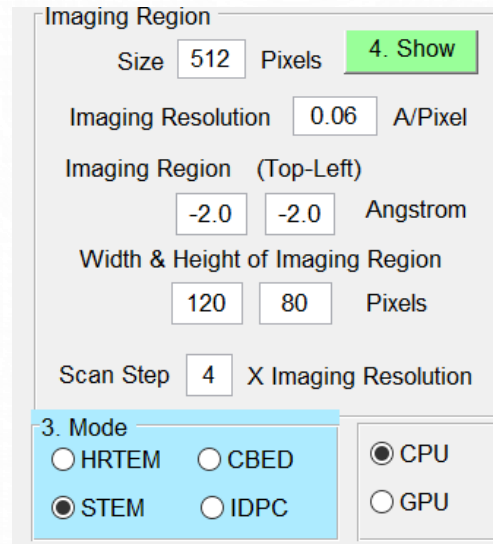
> Green box: region of the calculated potential, determined by the red and black regions

> 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.

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HRTEM Model
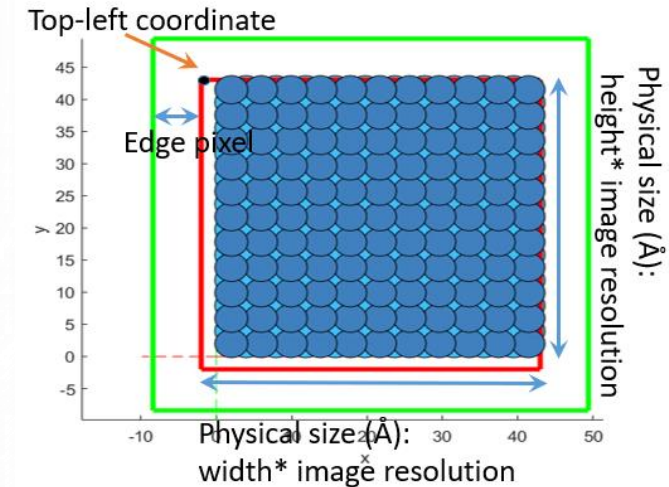
- ➢ Green box: region of the calculated potential, determined by the red region and its edge, e.g. the side length is (512+64*2)

- ➢ '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
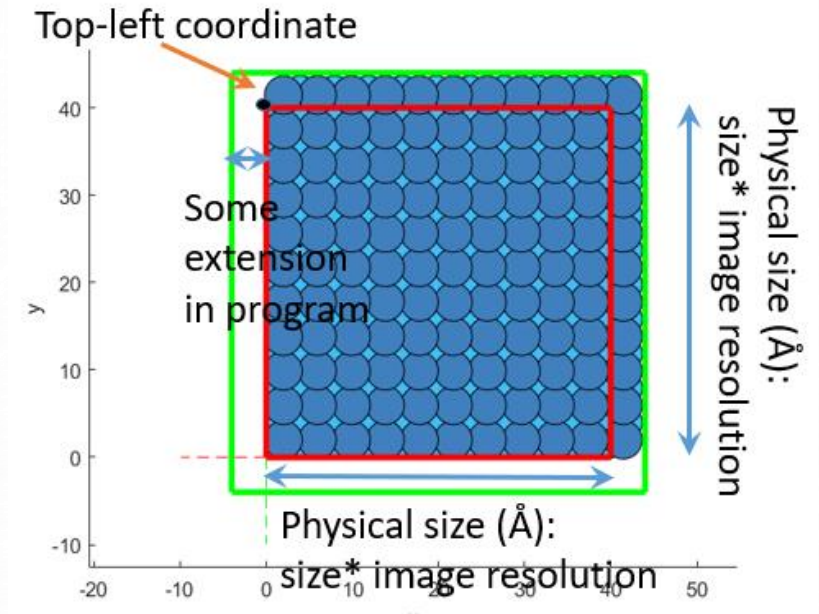
> Green box: region of the calculated potential, and it is extended by a constant (4 Angstrom) to eliminate the aliasing.

> 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'.
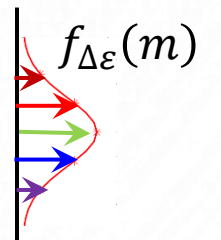
3.3 Coherence

Imaging Condition

Voltage: 200 kV   Aperture 10 1/nm
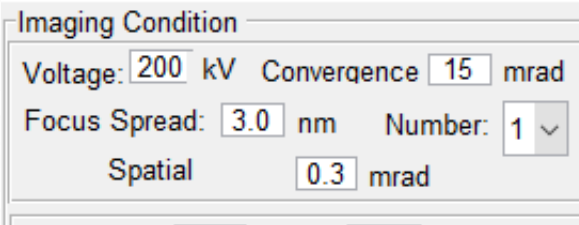Focus Spread: 3.0 nm   Number: 1
Spatial Convergence: 0.3 mrad

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

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

$f_{\Delta\varepsilon}(m)$

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:
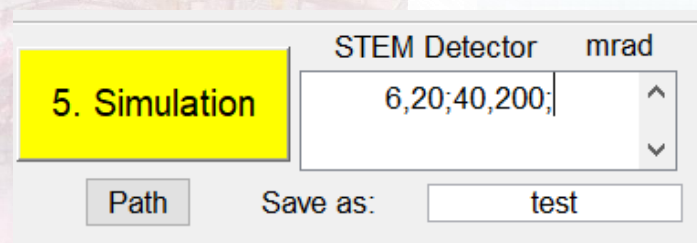
$$\chi(k, \Delta f, A_1, A_2, B_2, \dots) = Re\left\{\frac{1}{2}\Delta f \lambda k k^* + \frac{1}{2}A_1\lambda k^{*2} + \right.$$
$$\frac{1}{3}A_2 k^2 k^{*3} + B_2\lambda^2 k^2 k^* + \frac{1}{4}Cs\lambda^3(kk^*)^2 + \frac{1}{4}A_3\lambda^3 k^{*4} +$$
$$S_3\lambda^3 k^3 k^* + \frac{1}{5}A_4\lambda^4 k^{*5} + D_4\lambda^4 k^4 k^* + B_4\lambda^4 k^3 k^{*2} +$$
$$\left.\frac{1}{6}C_5\lambda^5(kk^*)^3 + \frac{1}{6}A_5\lambda^5 k^{*6} + R_5\lambda^5 k^5 k^* + S_5\lambda^5 k^4 k^{*2}\right\} =$$
$$\frac{1}{2}\Delta f \lambda k k^* + \frac{1}{4}Cs\lambda^3(kk^*)^2 + \chi'(k, A_1, A_2, B_2, \dots)$$

A_ξ θ_ξ

	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 aberration S3:	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
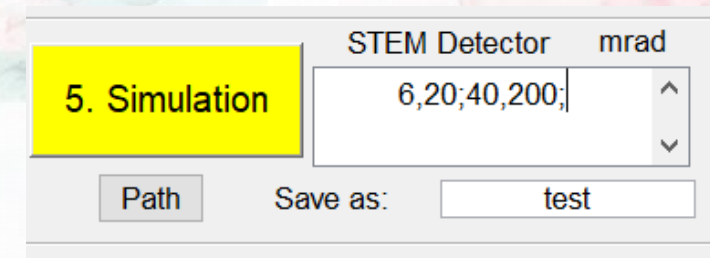
3.5 Detectors

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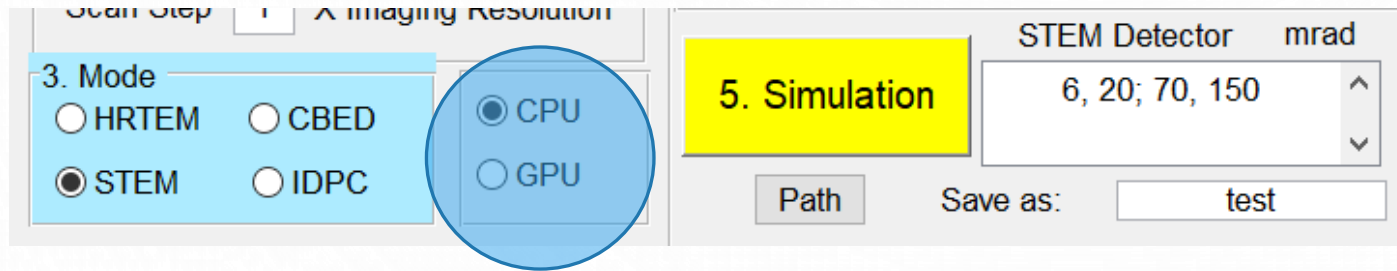
➢**IDPC modes**: The Angle of the detector is separated by ',' , 6 is inner angle and 20 is exterior angle. And different detectors is separated by ';'.

STEM Detector   mrad

5. Simulation   6,20;40,200;

Path   Save as: test

STEM Detector   mrad

5. Simulation   6,20;40,200;

Path   Save as: test

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.

2. Crystal

Filename | mp-5229_SrTiO3101025.p

Output | 1,10 | **2. Slicing**

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

Intensity profile of Probe Wave
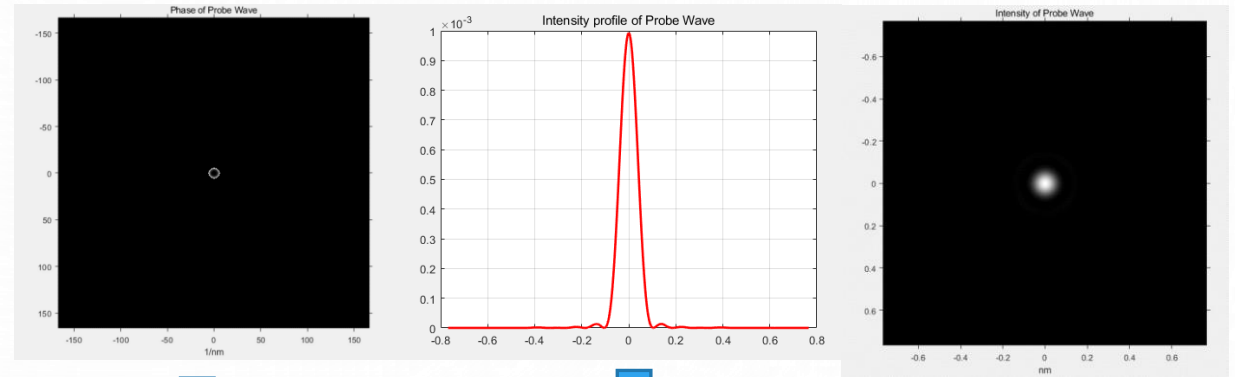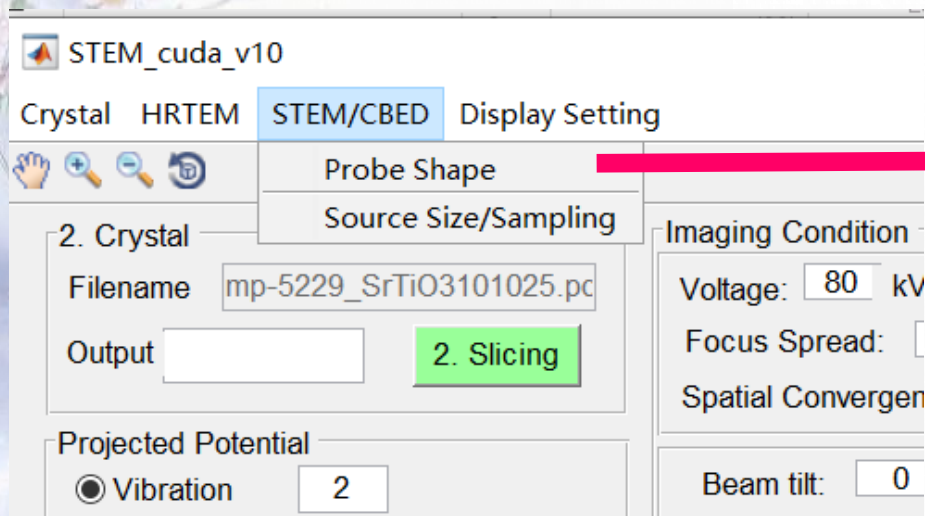
Phase of probe wave

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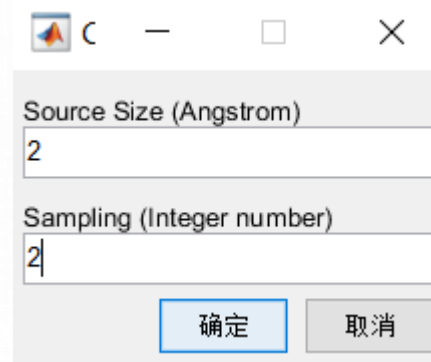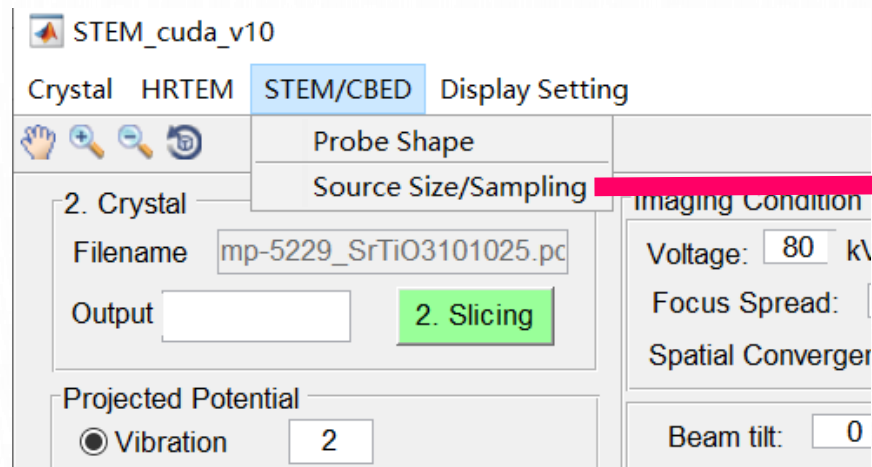
Result
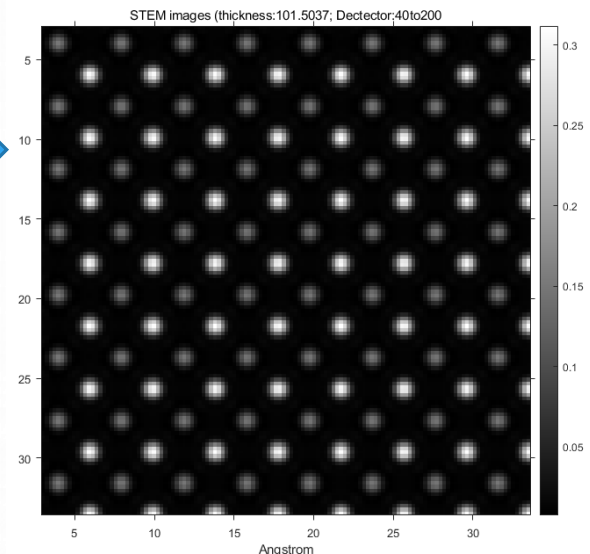
Blurred image
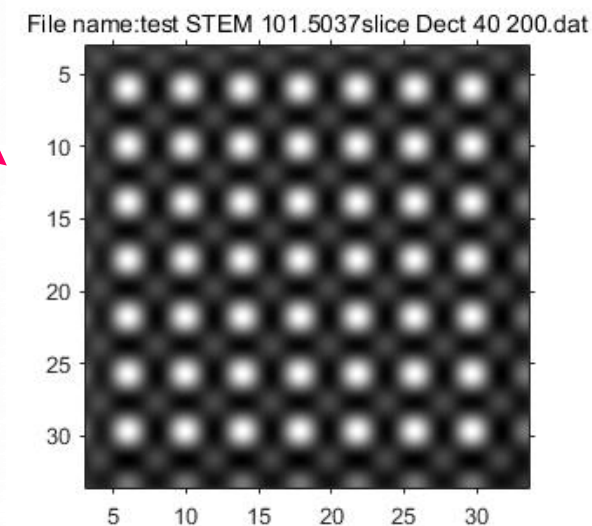
The STEM image can be blurred by a Gaussian function with a specified full width at half maxima (FWHM) and increasing the sampling, which is designed with reference to QSTEM.

4.2HRTEM related
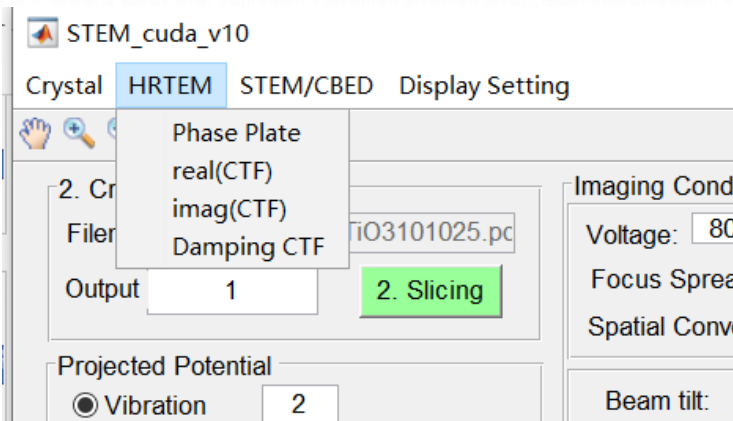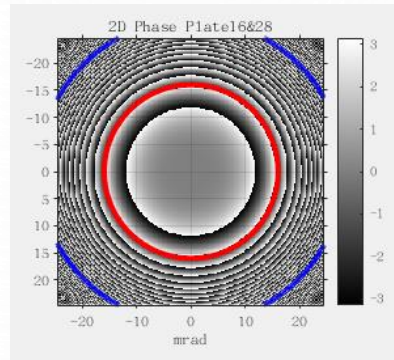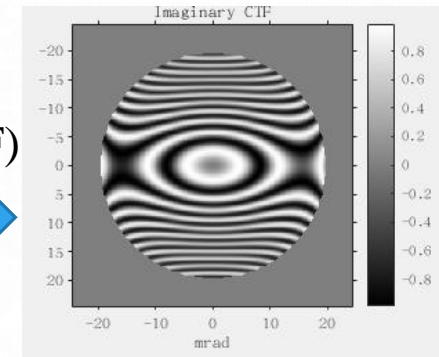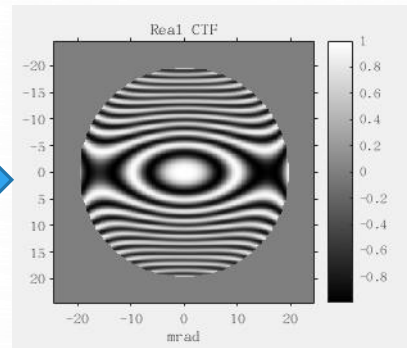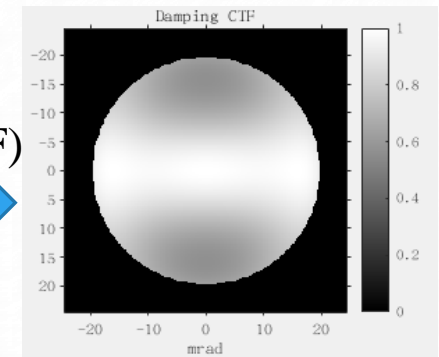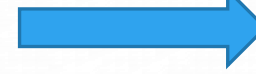
4.3 Save the file

Select the folder to store the results
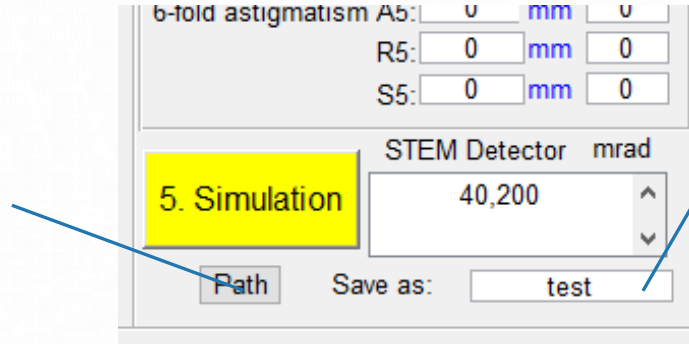
Name of result

The result will be named as test_STEM_101.5037slice_Dect_40_200.dat
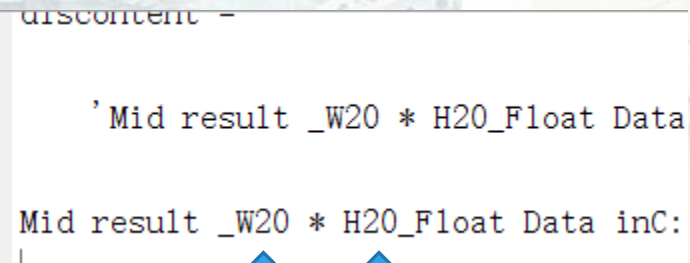
name model thickness Detector angle

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';

discontent =

　　　'Mid result _W20 * H20_Float Data

Mid result _W20 * H20_Float Data inC:

Size: Output at the end of the program

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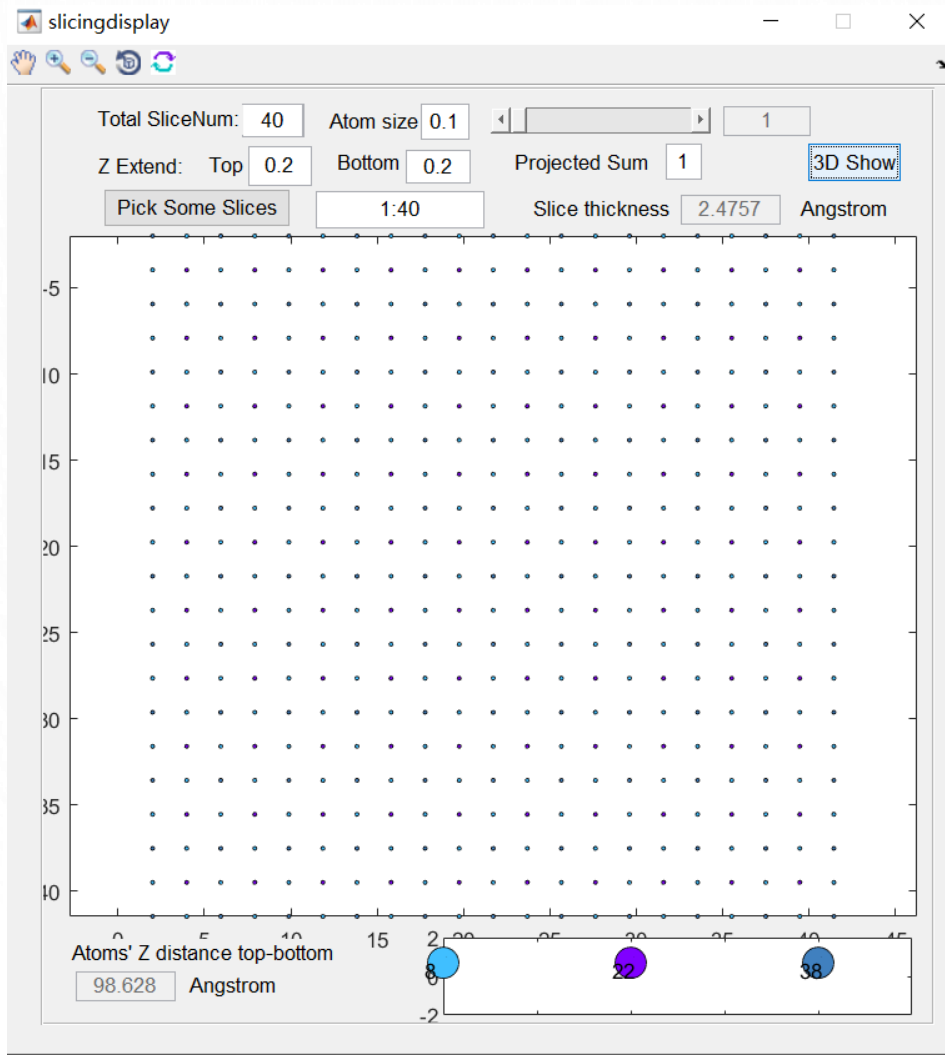
The simulation uses the $SrTiO_3$, the pictures is the slicing interface parameter setting, The slicing interface settings of all modes are the same. The interface parameter settings of different modes are different, and they will be given in different modes. The parameters of the potential calculation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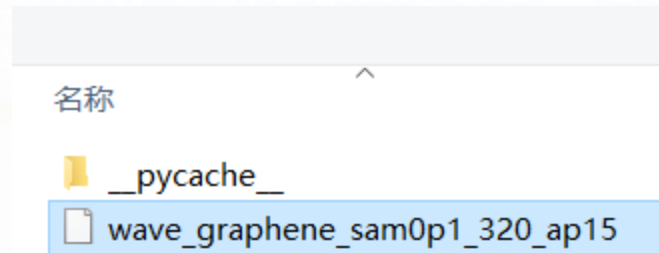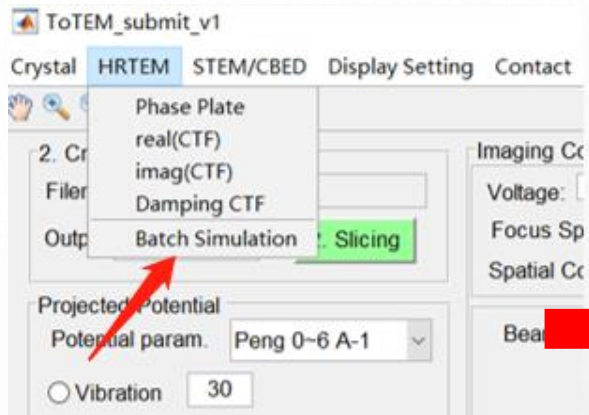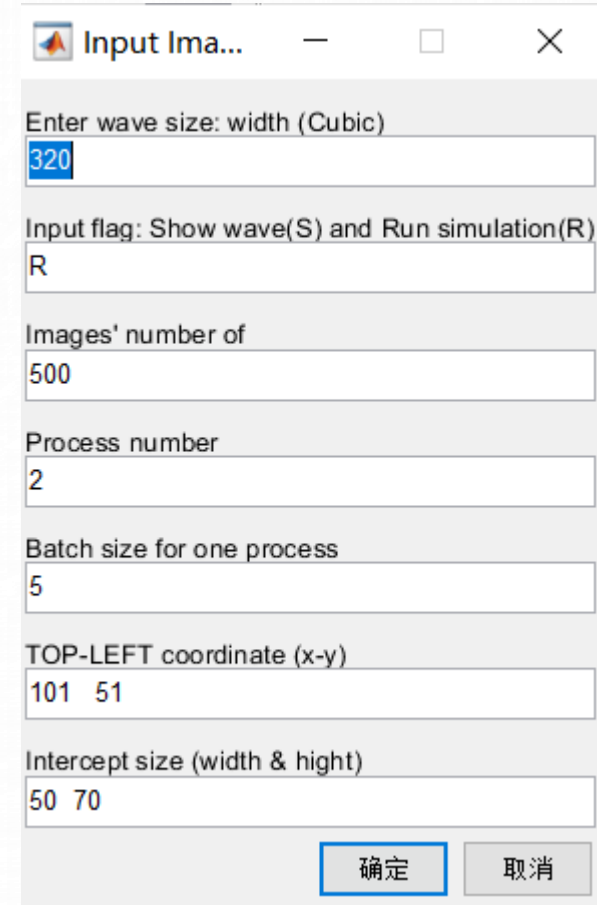
5.1 HRTEM

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

ToTEM_submit_v1
Crystal HRTEM STEM/CBED Display Setting Contact

Phase Plate
real(CTF)
imag(CTF)
Damping CTF
Batch Simulation

Imaging Co
Voltage:
Focus Sp
Spatial Co

Projected Potential
Potential param. Peng 0~6 A-1
○ Vibration 30

Bea

名称

__pycache__
wave_graphene_sam0p1_320_ap15

Exit wave function
generated in HRTEM mode

Input Ima... — □ ×

Enter wave size: width (Cubic)
320

Input flag: Show wave(S) and Run simulation(R)
R

Images' number of
500

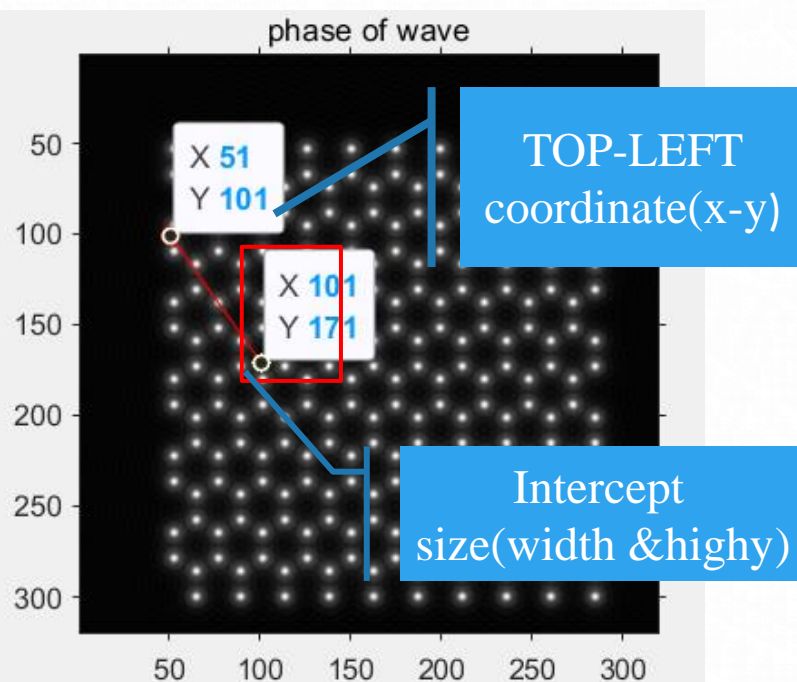Process number
2

Batch size for one process
5

TOP-LEFT coordinate (x-y)
101 51

Intercept size (width & hight)
50 70

确定 取消

Run simulation(R): start to generate images

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

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

phase of wave

X 51
Y 101

X 101
Y 171

TOP-LEFT coordinate(x-y)

Intercept size(width &highy)

Input Ima... — □ ✕

Enter wave size: width (Cubic)
320

Input flag: Show wave(S) and Run simulation(R)
R

Images' number of
500

Process number
2

Batch size for one process
5

TOP-LEFT coordinate (x-y)
101 51

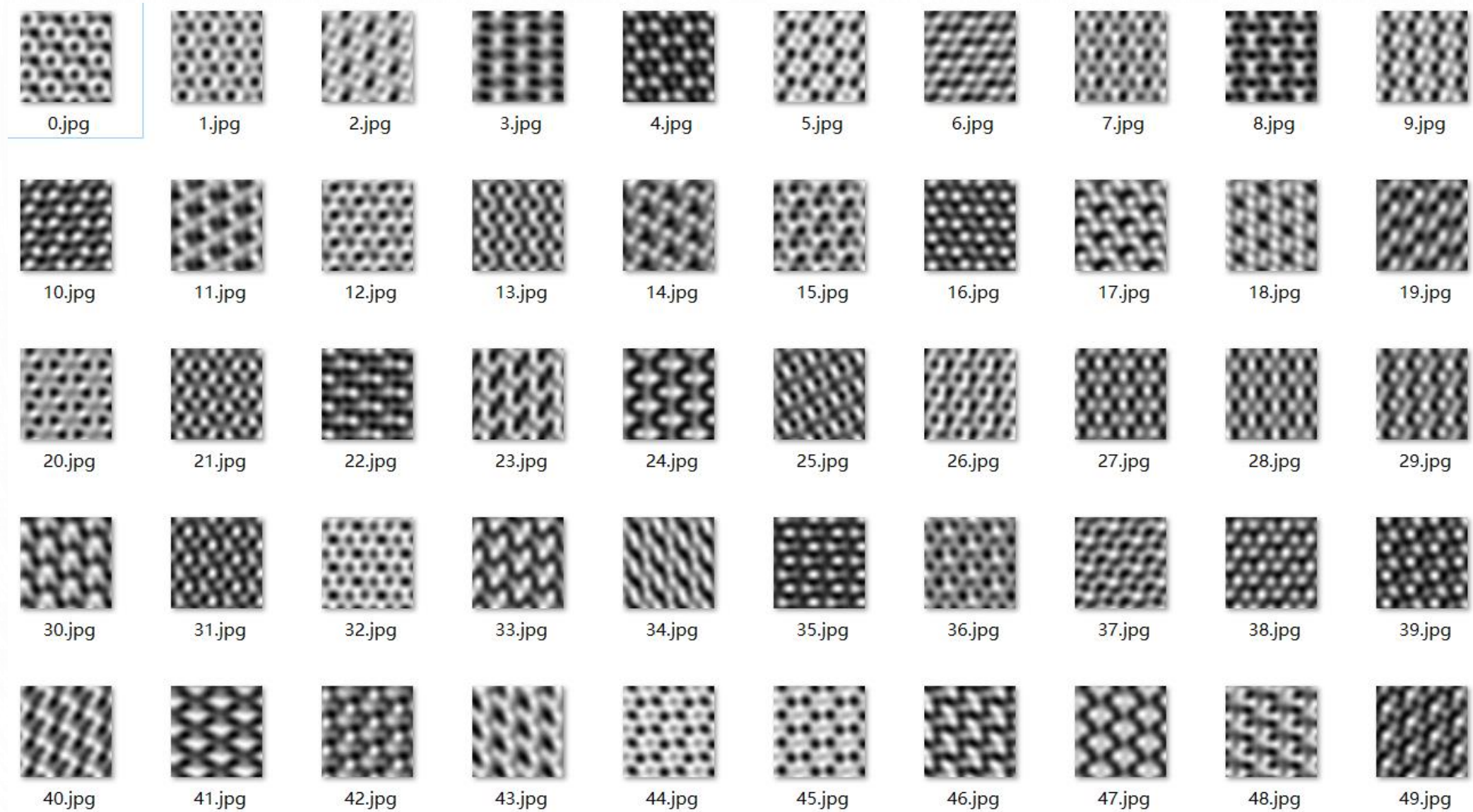Intercept size (width & hight)
50 70

确定   取消

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。

📁 [0]
📁 __pycache__
📄 parameter_batchsimulation
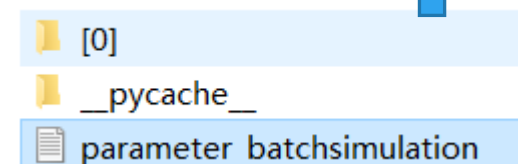
Import ranges to randomly generate values around each aberration.

	Magnitude(nm) & Angle(degree)		
Beam tilt:	0	mrad	0 degree
Defocus C1:	-2.5	nm	
2-fold astigmatism A1:	2.5	nm	0
3-fold astigmatism A2:	40	nm	0
Axial coma B2:	35	nm	0
(C3) Cs:	4	um	
4-fold astigmatism A3:	0.8	um	0
Axial star aberrationS3:	0.8	um	0
5-fold astigmatism A4:	50	um	-130.9
3-lobe aberration D4:	32.4	um	112.1
coma B4:	60	um	0
C5:	2.71	mm	
6-fold astigmatism A5:	2.562	mm	-65.9
R5:	0	mm	0
S5:	0	mm	0

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Batch simulation result

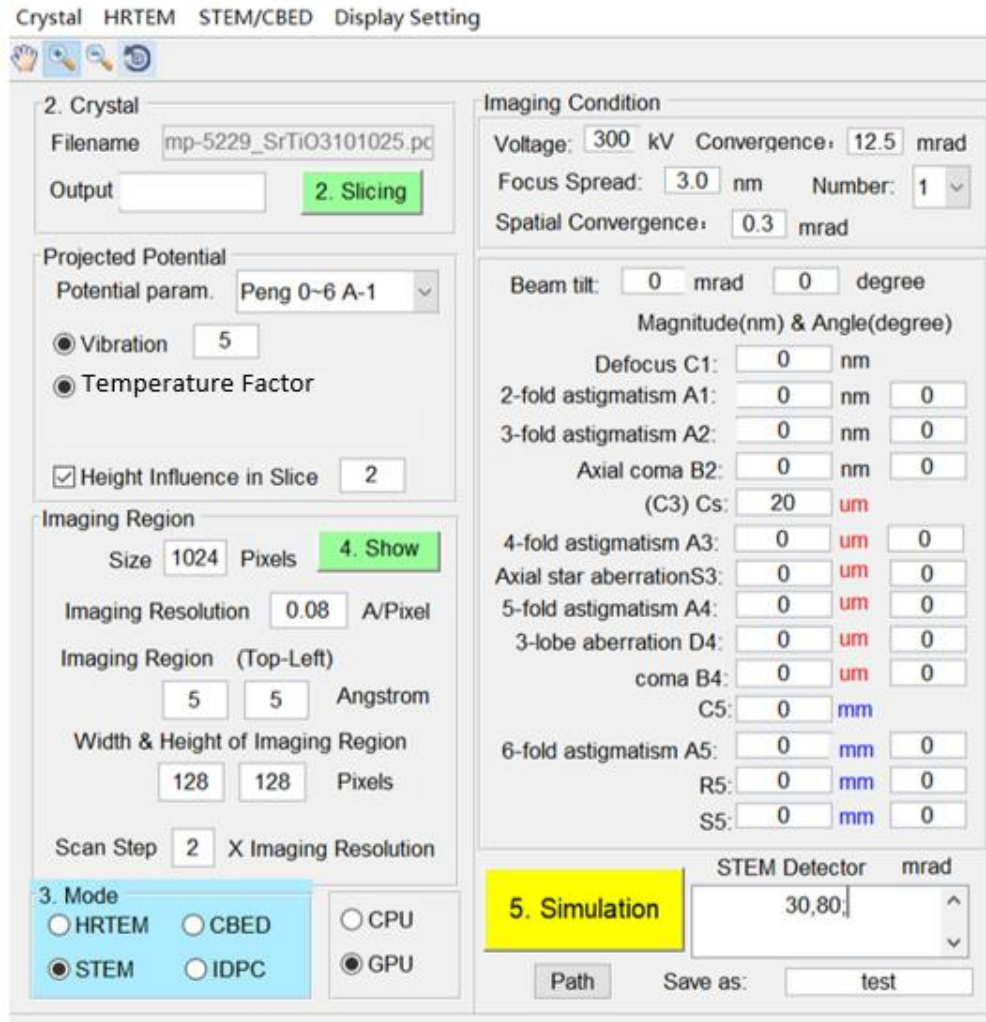Fifty images of HRTEM model were successfully generated!

5.2 CBED

interface

result

5.3 STEM

Thickness is 101.5037Å

interface
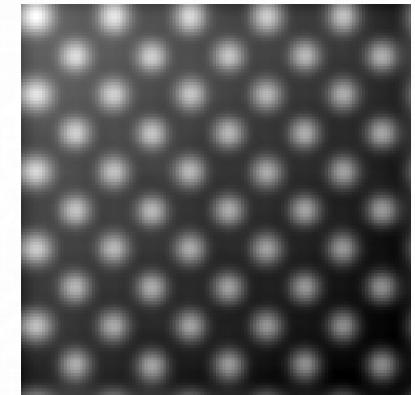
result

blurred by Gaussian Function
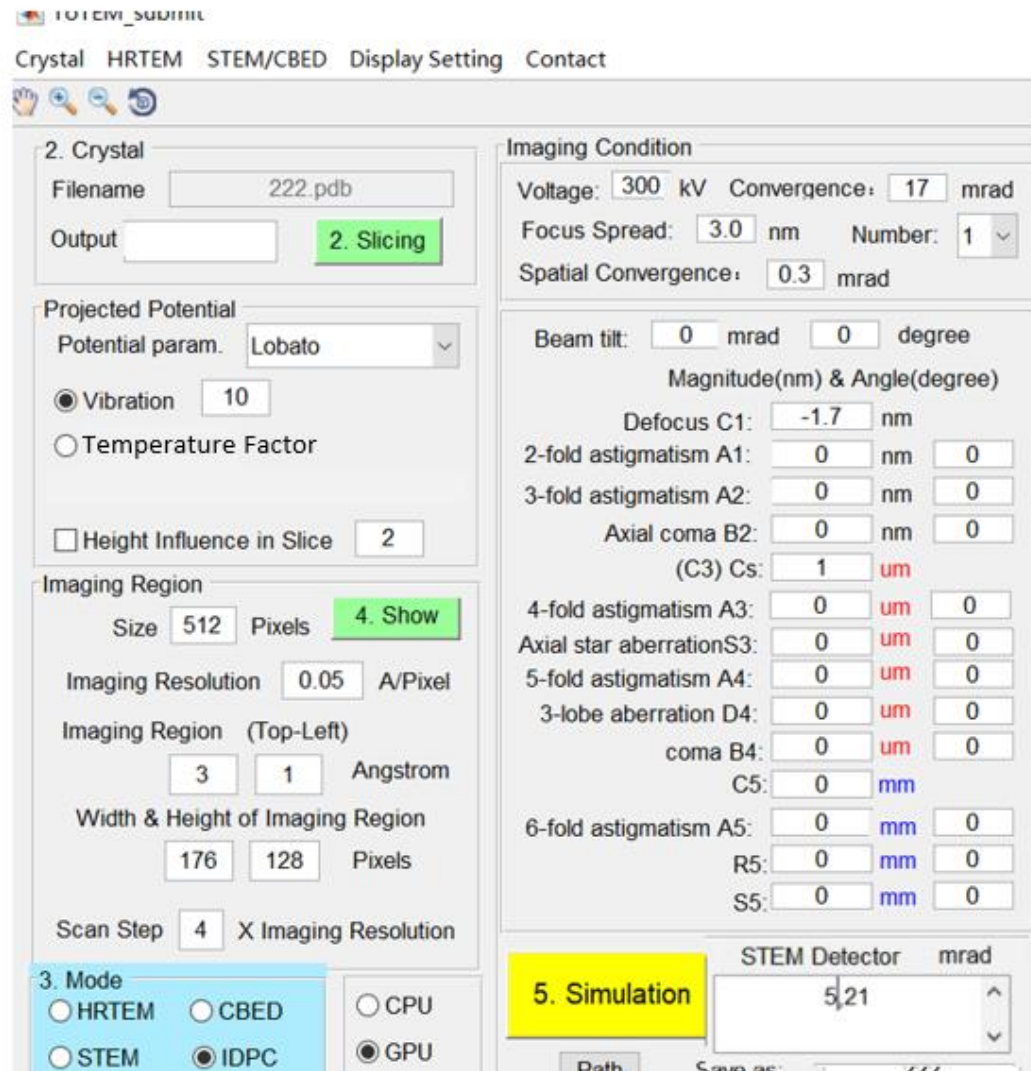
5.4 IDPC

Thickness is 23.7Å

interface

result

blurred by Gaussian Function

5.5 IDPC Simulation for MFI-type zeolites

Thickness is 38.3Å

interface
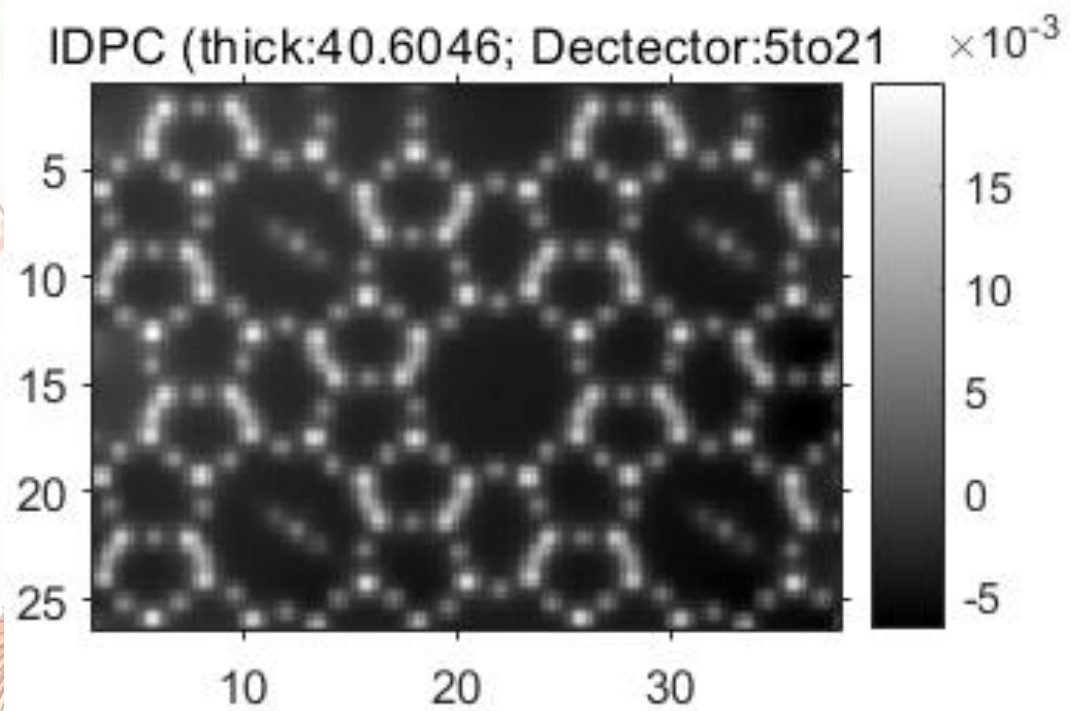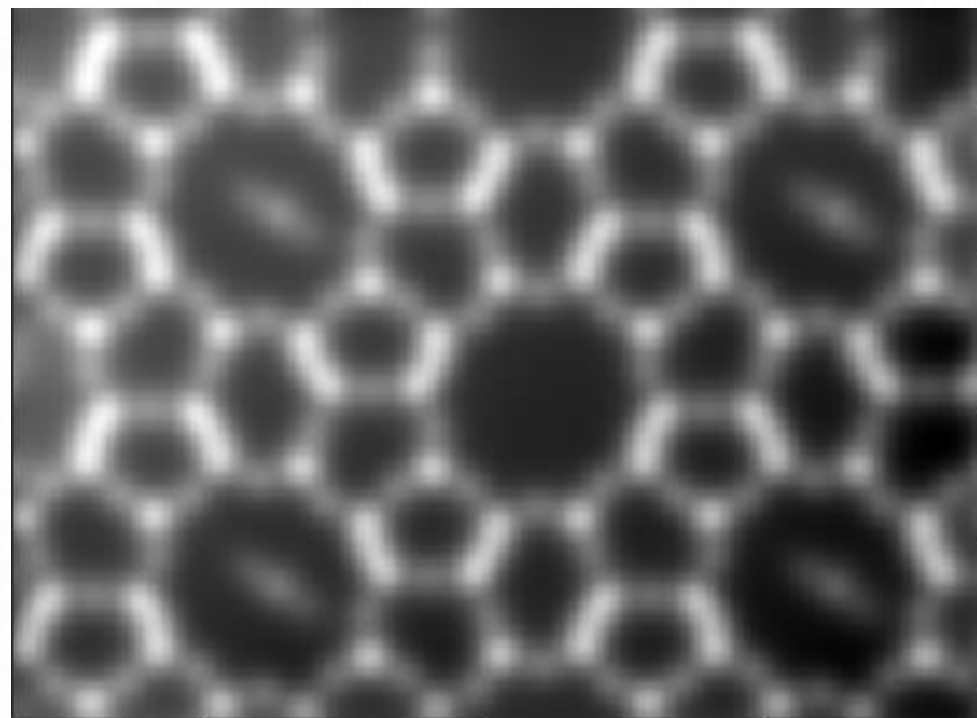
Structure

010 direction

result

blurred by Gaussian Function

IDPC (thick:40.6046; Dectector:5to21) ×10⁻³

Thank you for using ToTEM