SPaMD_Visualizer_manual

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1 Model Part

1.1 Monocrystall

1.1.1 cF4[225]-A1(Cu) Monocrystall

Main Process：

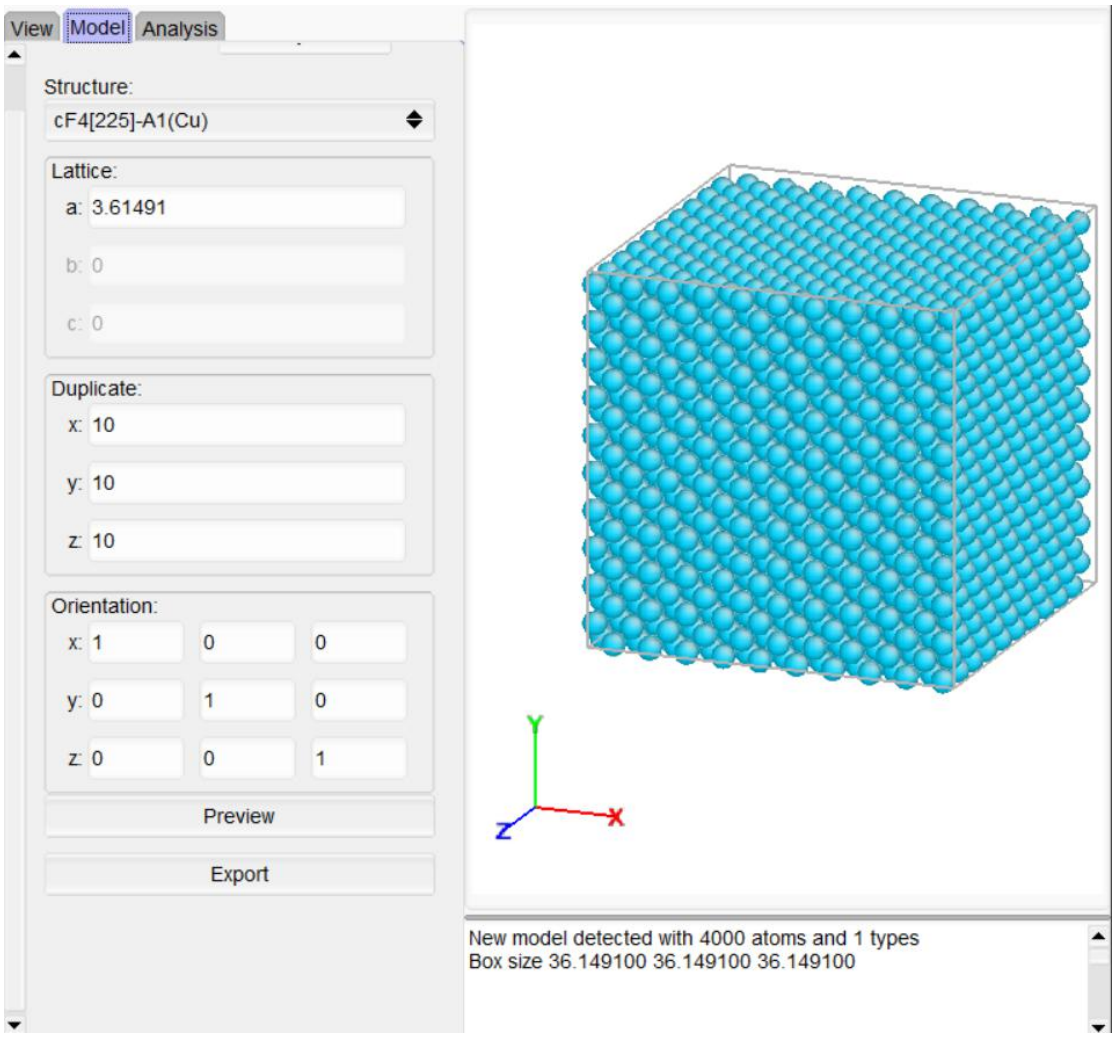
① Select Monocrystall Modelling _Select model

② Select cF4[225]-A1(Cu)_Structure，lattice parameters_Lattice

③ Setting expansion times:10_Duplicate

④ Setting crystal orientation _Orientation

⑤ Preview or Export



1.2 Polycrystal

1.2.1 cF4[225]-A1(Cu) Polycrystal

Main Process：

① Choosing Polycrystall Modelling_Select model

② Setting Lattice Parameter 200Å_x、_y、_z

③ Setting Lattice Gap 0. 1Å_Cutoff

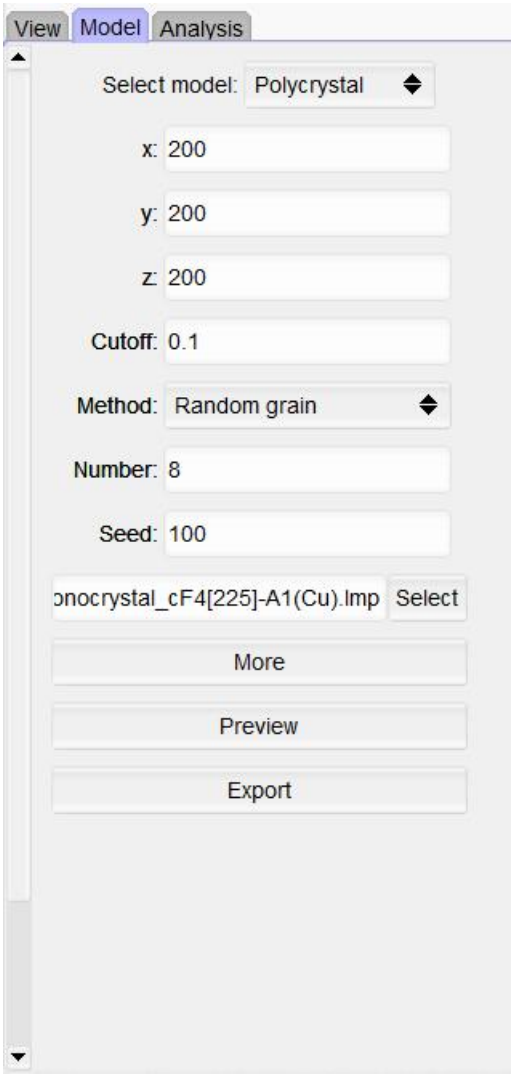
④ Choosing grain distribution pattern:Random Grain_Method

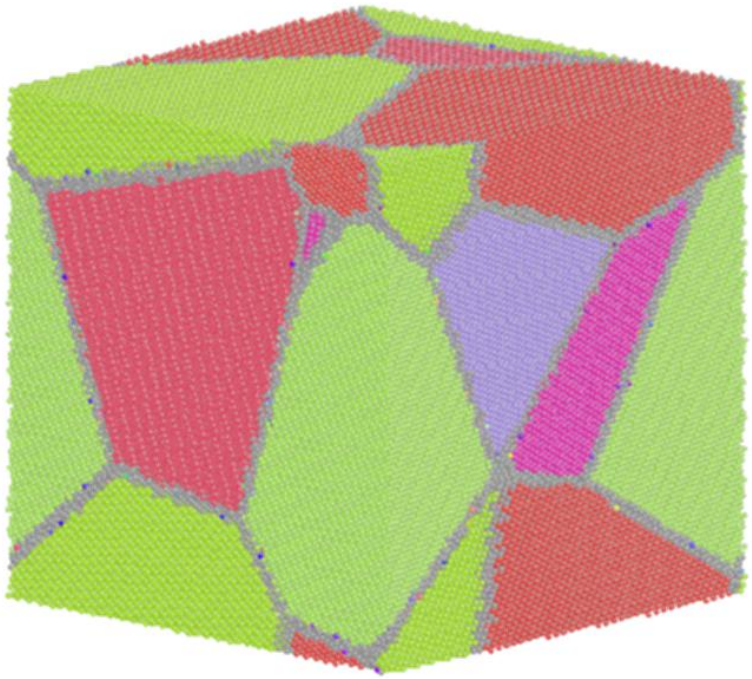
⑤ Setting the number of grains:8_Number

⑥ Setting the number of random seeds:100_Seed

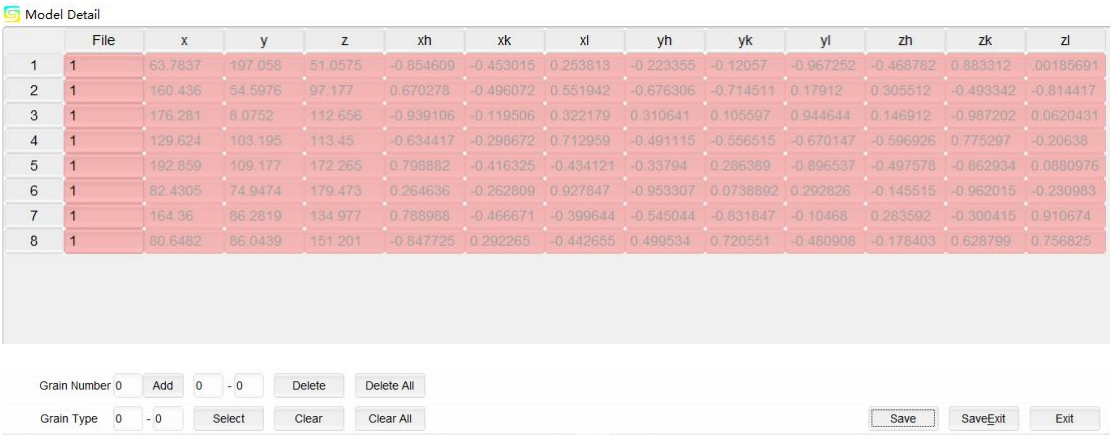
⑦ Read cF4[225]-A1(Cu) monocrystal file_Select

⑧ Preview or Export





⑨ For the generated polycrystalline file, see the detail interface for the grain number, source file, position and orientation information _More



⑩ Setting the number of grains:2_Grain Number，clicking Add，for adding more 2 grains in the former model.Enter 2-4 in the left table and click Delete to delete the grains in 2-4.Enter 2-2 in the bottom table_Grain Type and click Clear to clear the information of grain .The former operation only take effect when Save or Save_Exit.

Model Detail

	File	x	y	z	xh	xk	xl	yh	yk	yl	zh	zk	zl
1	1	63.7837	197.058	51.0575	-0.854609	-0.453015	0.253813	-0.223355	-0.12057	-0.967252	-0.468782	0.883312	.00185691
2	1	160.436	54.5976	97.177	0.670278	-0.496072	0.551942	-0.676306	-0.714511	0.17912	0.305512	-0.493342	-0.814417
3	1	176.281	8.0752	112.656	-0.939106	-0.119506	0.322179	0.310641	0.105597	0.944644	0.146912	-0.987202	0.0620431
4	1	129.624	103.195	113.45	-0.634417	-0.298672	0.712959	-0.491115	-0.556515	-0.670147	-0.596926	0.775297	-0.20638
5	1	192.859	109.177	172.265	0.798882	-0.416325	-0.434121	-0.33794	0.286389	-0.896537	-0.497578	-0.862934	0.0880976
6	1	82.4305	74.9474	179.473	0.264636	-0.262809	0.927847	-0.953307	0.0738892	0.292826	-0.145515	-0.962015	-0.230983
7	1	164.36	86.2819	134.977	0.788988	-0.466671	-0.399644	-0.545044	-0.831847	-0.10468	0.283592	-0.300415	0.910674
8	1	80.6482	86.0439	151.201	-0.847725	0.292265	-0.442655	0.499534	0.720551	-0.480908	-0.178403	0.628799	0.756825
9	1	151.469	37.6415	159.941	-0.852858	0.161948	-0.496393	0.0613893	-0.91299	-0.403337	-0.518522	-0.374462	0.768709
10	1	151.653	193.329	135.984	0.475993	0.730776	-0.489282	0.456948	0.269847	0.847573	-0.751418	0.627016	0.205481

Model Detail

	File	x	y	z	xh	xk	xl	yh	yk	yl	zh	zk	zl
1	1	63.7837	197.058	51.0575	-0.854609	-0.453015	0.253813	-0.223355	-0.12057	-0.967252	-0.468782	0.883312	.00185691
2	1	192.859	109.177	172.265	0.798882	-0.416325	-0.434121	-0.33794	0.286389	-0.896537	-0.497578	-0.862934	0.0880976
3	1	82.4305	74.9474	179.473	0.264636	-0.262809	0.927847	-0.953307	0.0738892	0.292826	-0.145515	-0.962015	-0.230983
4	1	164.36	86.2819	134.977	0.788988	-0.466671	-0.399644	-0.545044	-0.831847	-0.10468	0.283592	-0.300415	0.910674
5	1	80.6482	86.0439	151.201	-0.847725	0.292265	-0.442655	0.499534	0.720551	-0.480908	-0.178403	0.628799	0.756825
6	1	151.469	37.6415	159.941	-0.852858	0.161948	-0.496393	0.0613893	-0.91299	-0.403337	-0.518522	-0.374462	0.768709
7	1	151.653	193.329	135.984	0.475993	0.730776	-0.489282	0.456948	0.269847	0.847573	-0.751418	0.627016	0.205481

Model Detail

	File	x	y	z	xh	xk	xl	yh	yk	yl	zh	zk	zl
1	1	63.7837	197.058	51.0575	-0.854609	-0.453015	0.253813	-0.223355	-0.12057	-0.967252	-0.468782	0.883312	.00185691
2	0	192.859	109.177	172.265	0.798882	-0.416325	-0.434121	-0.33794	0.286389	-0.896537	-0.497578	-0.862934	0.0880976
3	1	82.4305	74.9474	179.473	0.264636	-0.262809	0.927847	-0.953307	0.0738892	0.292826	-0.145515	-0.962015	-0.230983
4	1	164.36	86.2819	134.977	0.788988	-0.466671	-0.399644	-0.545044	-0.831847	-0.10468	0.283592	-0.300415	0.910674
5	1	80.6482	86.0439	151.201	-0.847725	0.292265	-0.442655	0.499534	0.720551	-0.480908	-0.178403	0.628799	0.756825
6	1	151.469	37.6415	159.941	-0.852858	0.161948	-0.496393	0.0613893	-0.91299	-0.403337	-0.518522	-0.374462	0.768709
7	1	151.653	193.329	135.984	0.475993	0.730776	-0.489282	0.456948	0.269847	0.847573	-0.751418	0.627016	0.205481

1.2.2 cF4[225]-A1(Cu) Polycrystal (Manual)

Main Process：

① Choosing grain distribution pattern:Manual _Method.The number of random seeds is 0 by default_Seed

Other settings is same with those in 1.2

② Choosing interface in detail_More and modify the orientation and distribution of grains manually

Model Detail

	File	x	y	z	xh	xk	xl	yh	yk	yl	zh	zk	zl
1	1	50	50	50	0.447015	0.829119	0.335766	-0.828209	0.241781	0.50558	0.338005	-0.504086	0.794764
2	1	150	50	50	-0.692745	-0.638688	0.334934	0.545886	-0.767879	-0.335217	0.471288	0.0493843	0.880596
3	1	50	150	50	0.0254657	0.967136	0.252979	-0.407931	-0.22098	0.885867	-0.912658	0.125757	-0.388897
4	1	50	50	150	-0.907939	-0.228737	0.351178	0.359653	.00495151	0.933073	0.215167	-0.973476	0.0777701
5	1	50	150	150	-0.763466	0.645079	0.031511	0.0168554	0.0288723	0.999441	-0.645628	-0.763571	-0.01117
6	1	150	50	150	-0.634061	-0.324269	0.702009	0.507283	0.510758	0.694111	0.583635	-0.796226	0.159356
7	1	150	150	50	0.260086	-0.941419	-0.214675	-0.29563	0.134013	-0.945856	0.919216	0.309468	-0.243456
8	1	150	150	150	0.512531	-0.627935	0.58567	-0.73983	-0.669144	0.0699939	-0.435849	0.397422	0.807522

③Preview or Export

1.3 Bilayers

1.3.1 cF4[225]-A1(Cu)/ cI2[229]-A2(W) Bilayers

Main Process：

① Select Bilayers Modelling_Select model

② Set the normal direction : X axis

③ Read the monopoly file for the upper layer and lower layer respectively :cF4[225]-A1(Cu).lmp and cI2[229]-A2(W).lmp_Select Model.

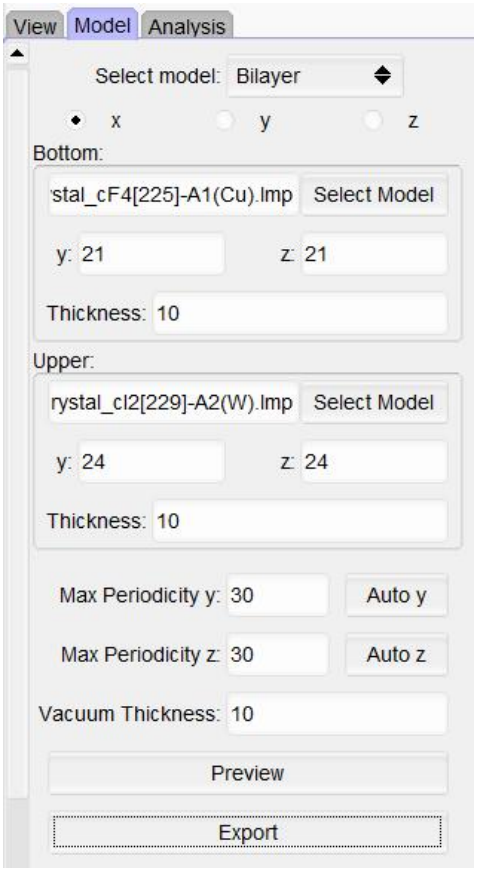
Set the thickness of layer:10Å_Thickness.as the length in the X direction.

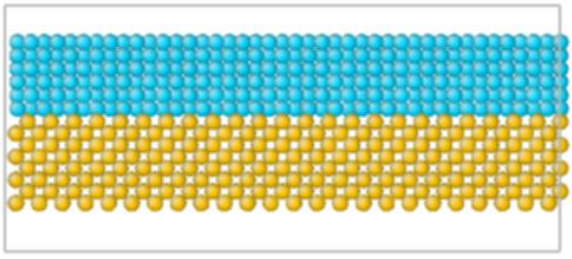
The gap of grain boundary has been set automatically

④ Set the max expansion times for 30 in Y and Z direction respectively: 30_Max Periodicity.

Click Auto to obtain the min expansion times for upper and lower layer in the Y and Z direction to match the size of upper and lower layer.

⑤ Set the thickness of vacuum layer:10 Å.(0 if not needed)





⑥ Preview or Export

1.4 Multilayer

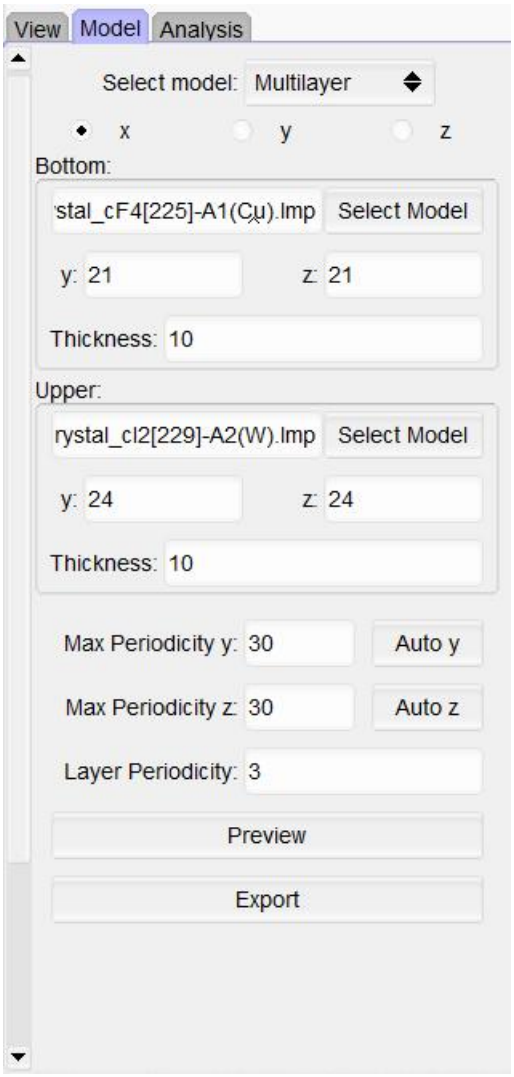
1.4.1 cF4[225]-A1(Cu)/ cI2[229]-A2(W) Multilayer

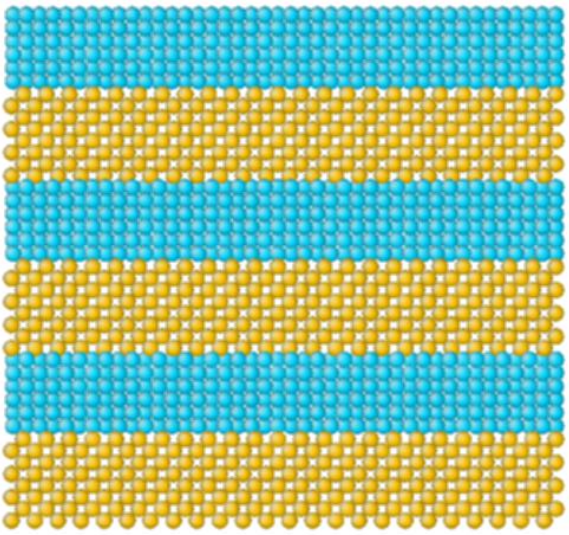
Main Process：

① Select Multilayer Modelling _Select model

② Set the expansion time:3_Layer Periodicity for other settings same with 1.3

③ Preview or Export





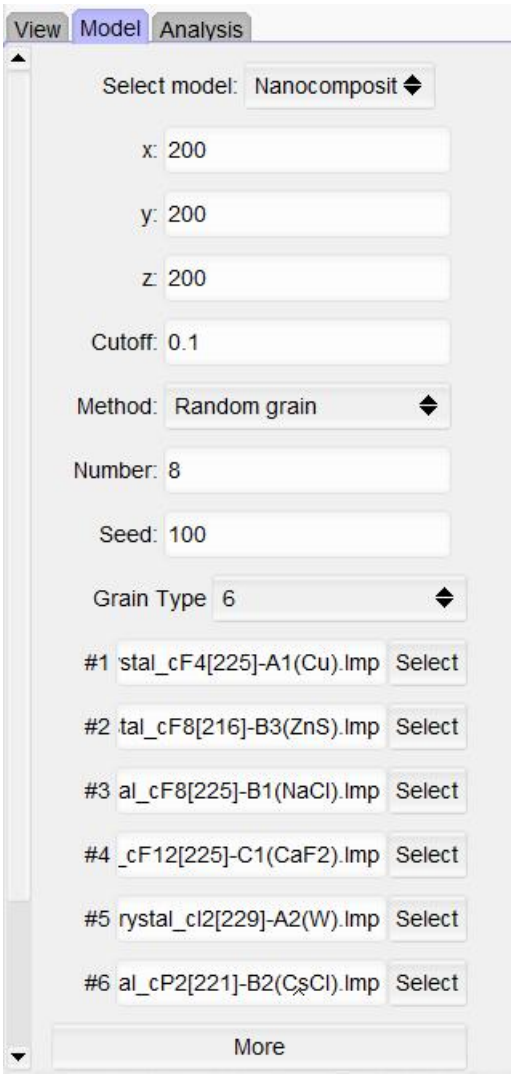
1.5 Nanocomposite

1.5.1 Nanocomposite

Main Process：

① Select Nanocomposite Modelling _Select model

② Set the number of grain types:6(max:6)_Grain Type and read 6 Monocrystal file _Select for the other settings same with 1.2



③ Users need to set the orientation and distribution of each grain type respectively in detail interface_More.

For example, enter 6-6 and Select the grain type :#6_Grain Type.

Click Select to set the sixth file for the NO.6 grain type

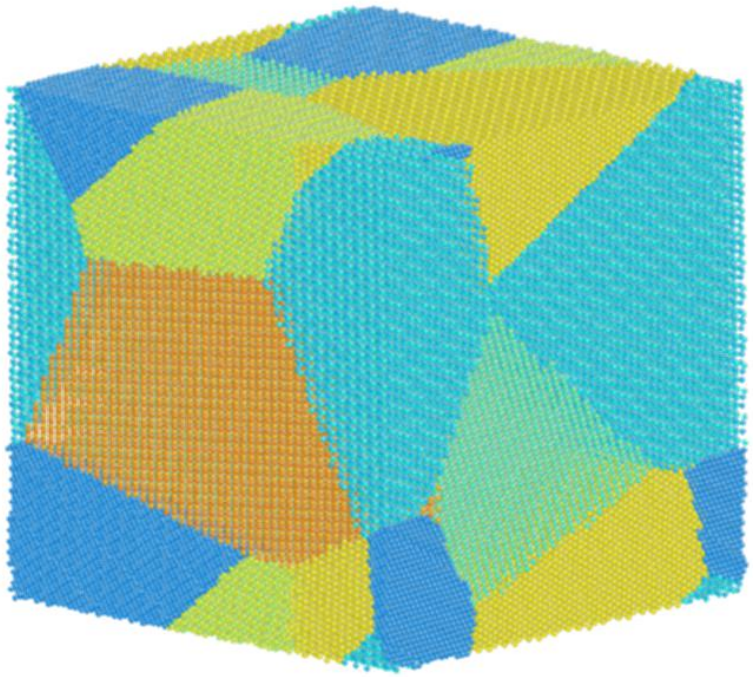
Model Detail

	File	x	y	z	xh	xk	xl	yh	yk	yl	zh	zk	zl
1	1	71.9749	197.497	176.141	0.571906	0.617975	0.539473	-0.346872	-0.413772	0.841708	-0.743373	0.668506	0.0222808
2	2	184.271	58.449	159.648	0.304329	0.83747	-0.453903	0.28588	-0.534838	-0.795123	-0.908656	0.112217	-0.402182
3	3	69.1794	126.695	102.841	-0.678836	0.696274	0.233203	-0.531151	-0.246327	-0.81068	0.507011	0.674185	-0.537043
4	4	86.5566	15.0822	179.211	-0.959498	0.169881	0.224732	-0.278477	-0.692564	-0.665436	0.0425963	0.701067	-0.711822
5	5	146.696	12.2806	134.581	0.841872	.00534452	-0.53965	-0.466347	0.496053	-0.732429	0.27161	0.868276	0.415121
6	6	92.8556	107.559	3.07016	0.993245	0.0264436	0.112986	-0.115355	-0.119407	0.986121	0.0125853	-0.992493	-0.12165

Grain Number 0 Add 0 - 0 Delete Delete All

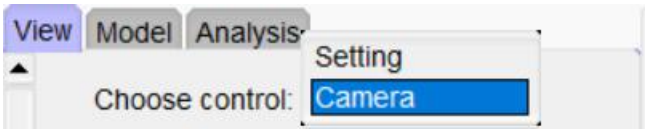
Grain Type #6 6 - 6 Select Clear Clear All Save SaveExit Exit

④ Preview or Export



2 View Part

（Take cF4[225]-A1(Cu) Nanocomposite as example）



2.1 Camera

Main Process：

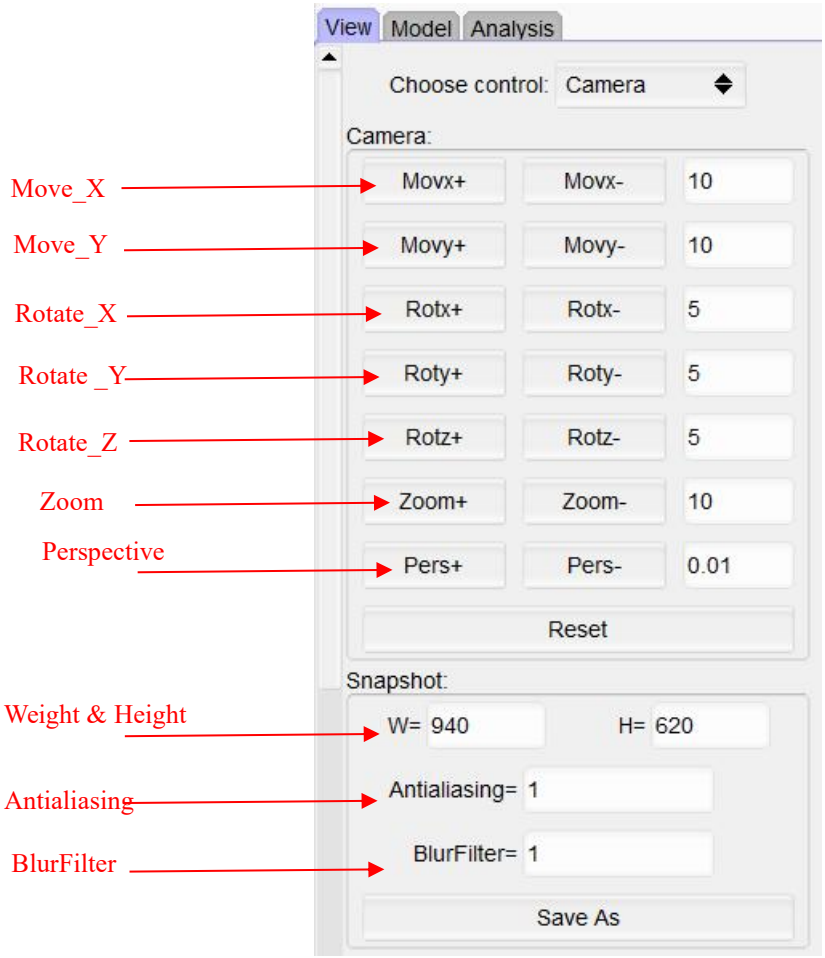
① Select the mode :Camera_Select control

② Users could click Mov、Rot、Zoom、Pers in the camera interface to control move,rotate,zoom,perspective

Click Reset to clear all the operations in the Camera interface

③ Users could set width and height of snapshot in the Snapshot interface and save the snapshot in the format of bmp,png or jpg

The current settings of snapshot is 940*620 with the format of png



2.2 Setting

Main Process：

① Select the control mode :Setting_Select control

② In the color bar,users need to set the coloring object including id、type、x、y、z and other data in the export file

In the RGB bars,users need to set coloring object for R,G,B value respectively

(Min :-4 Max :15)

③ Users could trim or delete in the Trimming interface with the center plane in the direction of three axes as the datum

Attention :Every time you click Cut, you will cut on the basis of the previous operation.

Click Recover to recover the status before the last trimming operation

④ Click Inverse to control inversely

Click Reset to clear all the operations expect those in the Trimming interface

⑤ Users could control atom radius in the Atom interface.

The currrent proportion is set to 1 as all types of atom keep their initial status

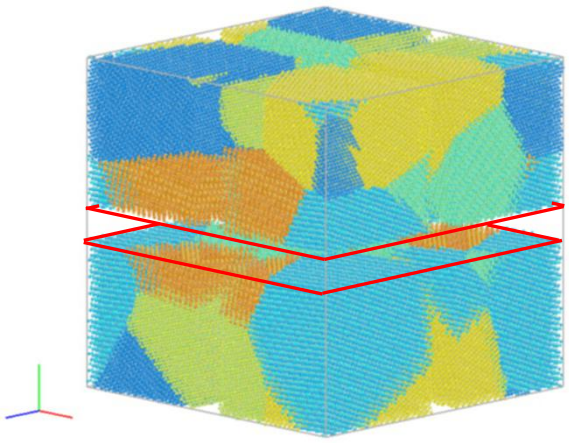
Click Rad to zoom

Click Chr to control the color brightness of atoms

Click Inspect Particle to retrieve data information in the previewing window

⑥ Control the frame of box /the color of backgraound/the three axes in the Box/Backgroud/Axes interfaces respectively

Coloring



Trimming in the direction of planes

Show Slice Region or not

Delete atoms with parameters between Min~Max

Relative atomic size

Size of atom

Atomic chroma（RGB）

View more information of atoms

Thickness of box

The color of background

Show axes or not

3 Analysis Part

3.1 Au Nanoindentation

3.1.1 CNA Analysis

Main Process：

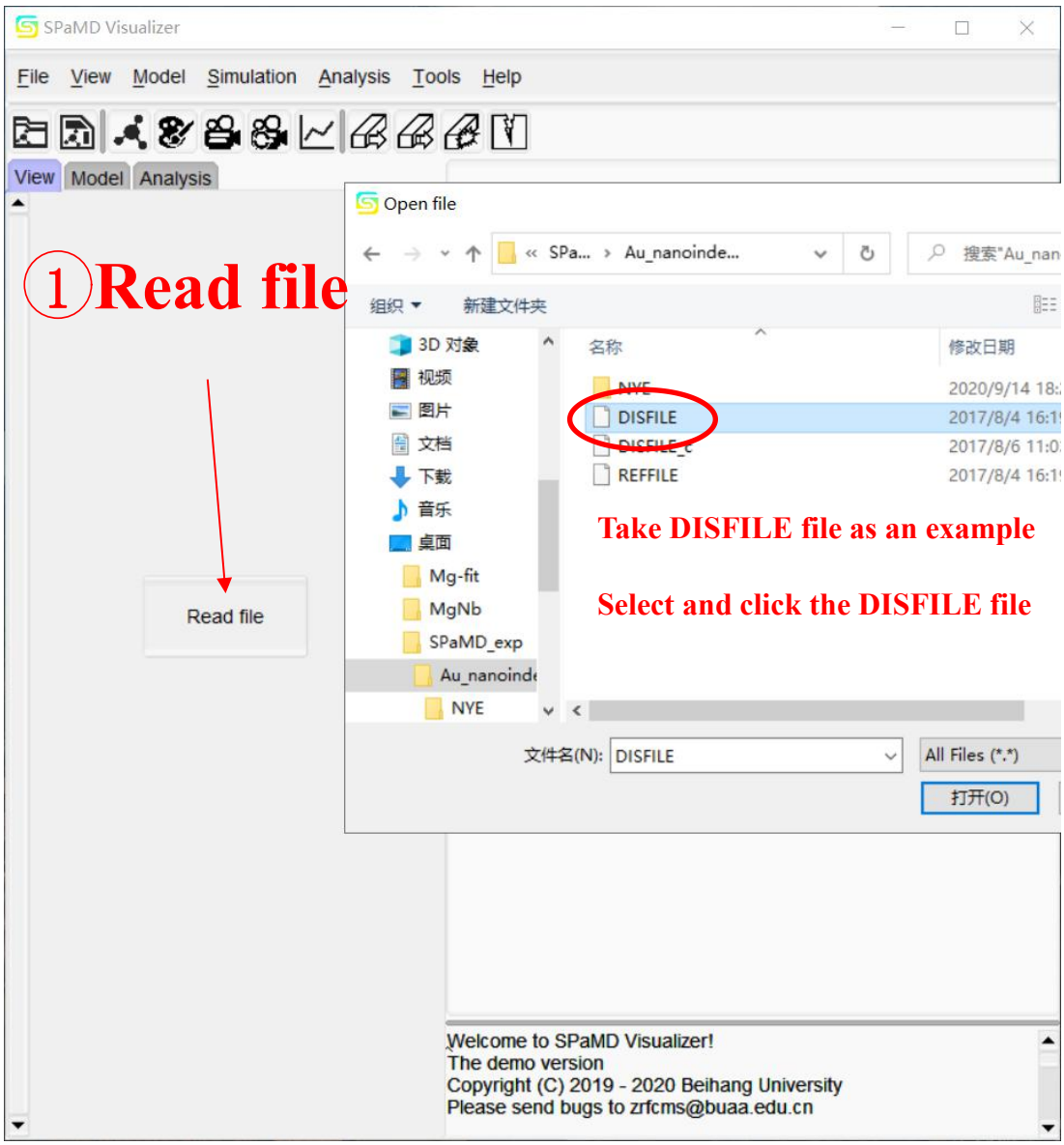
① Read monocrystal files_Read file

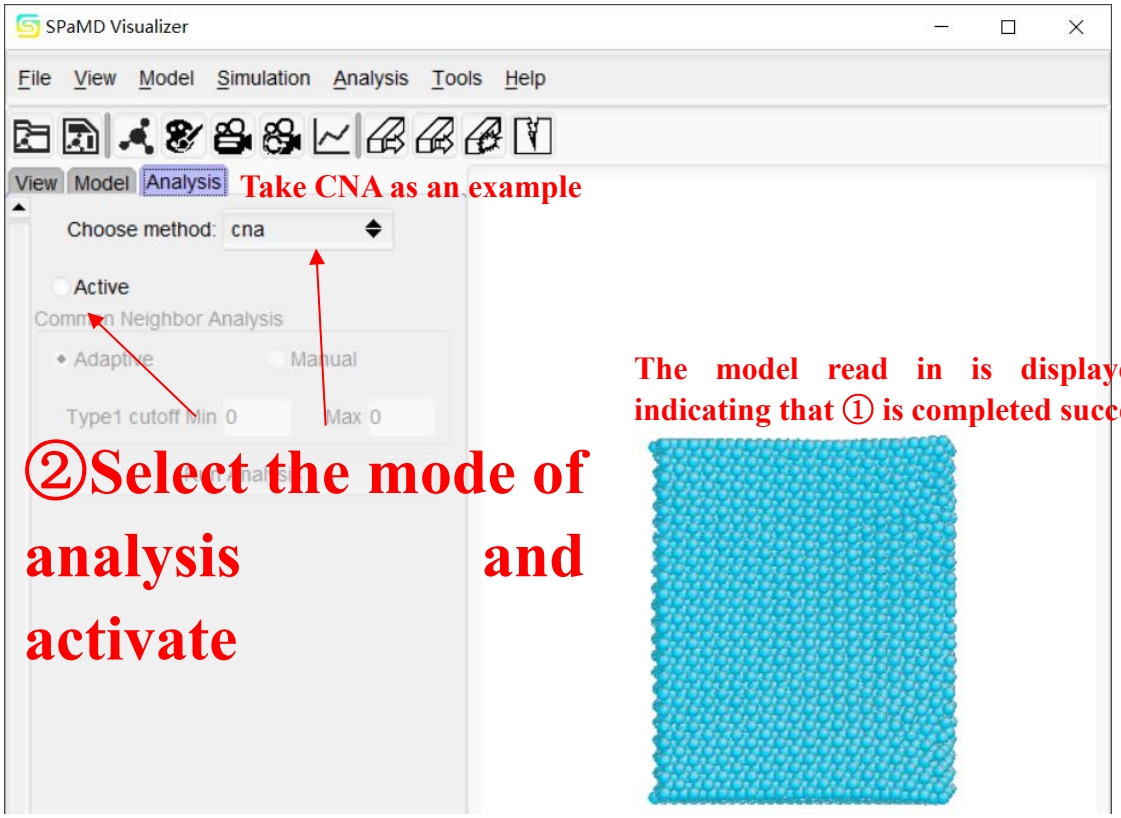
② Select the method of research_CNA and activate_Active

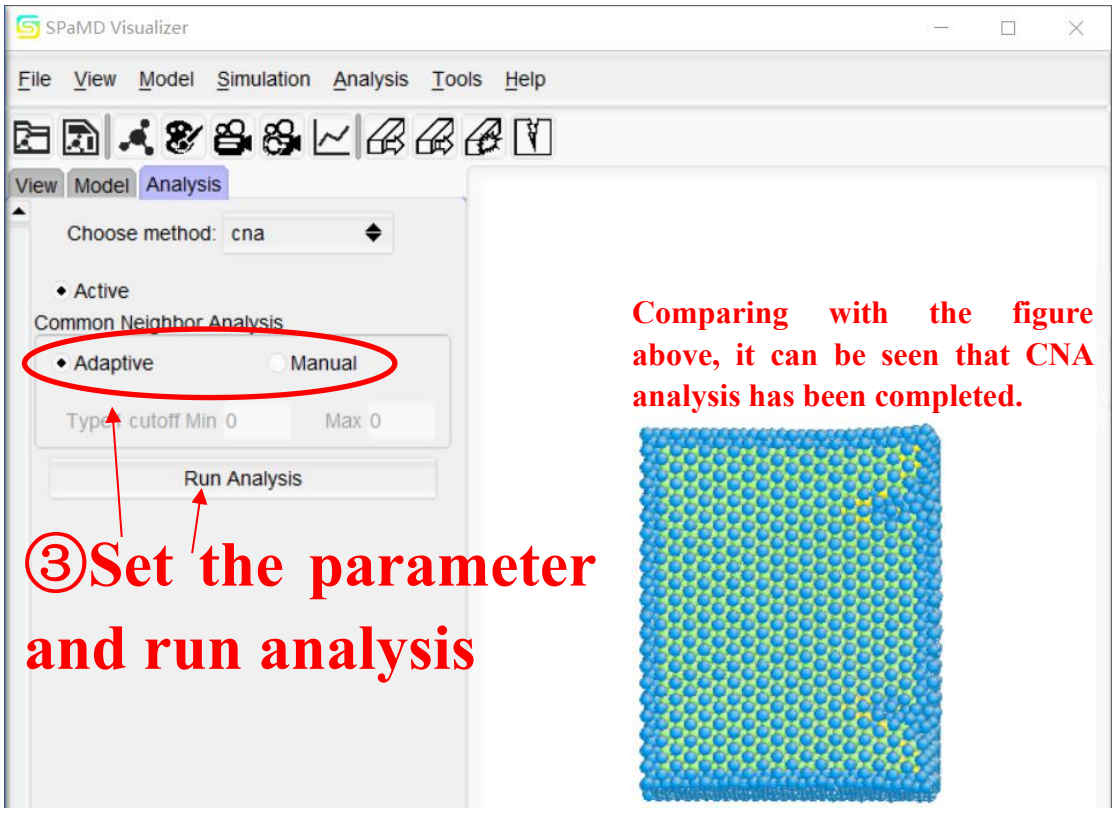
③ Set a series of parameters and click Run Analysis

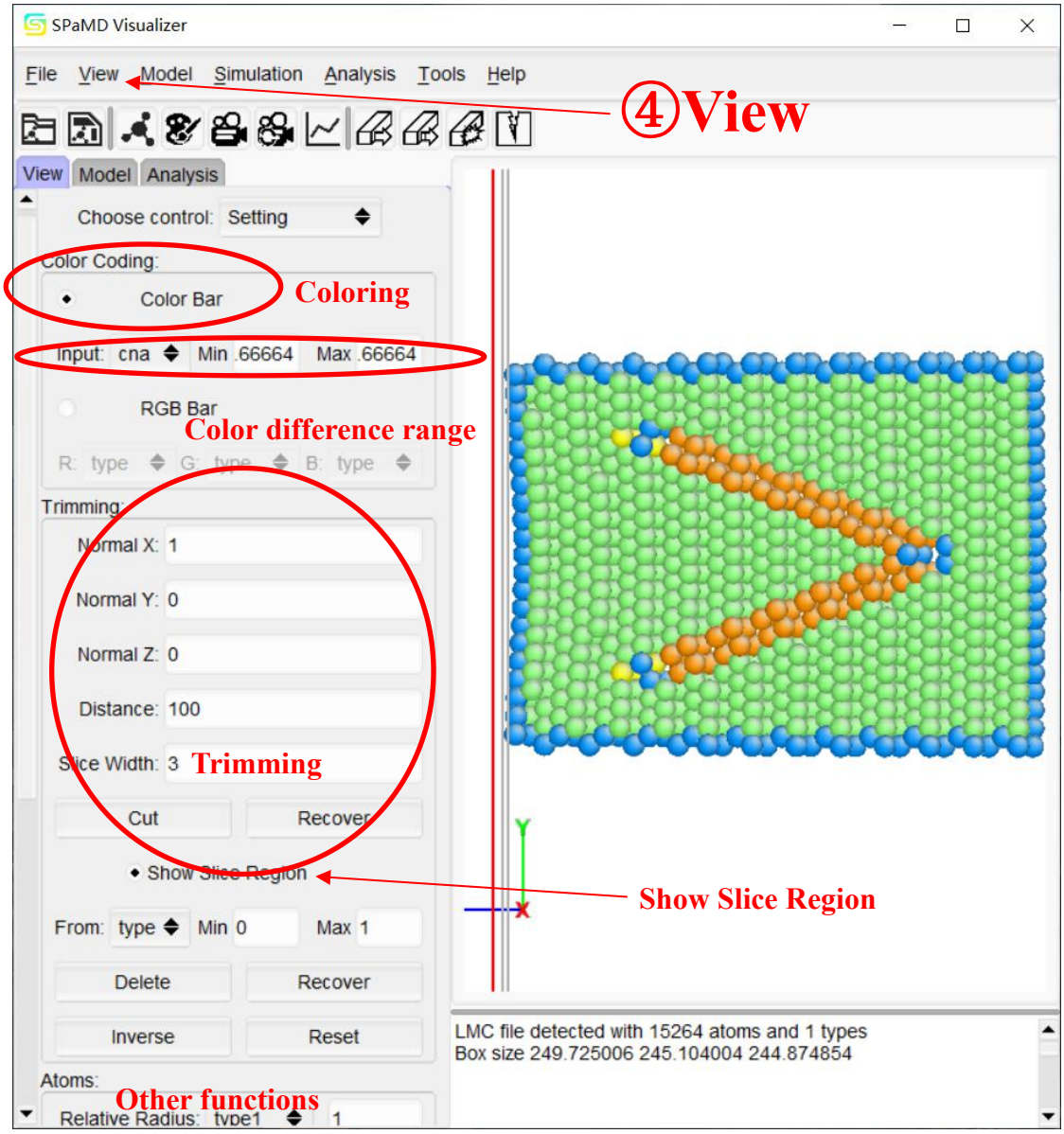
④ Click View to make a visual view

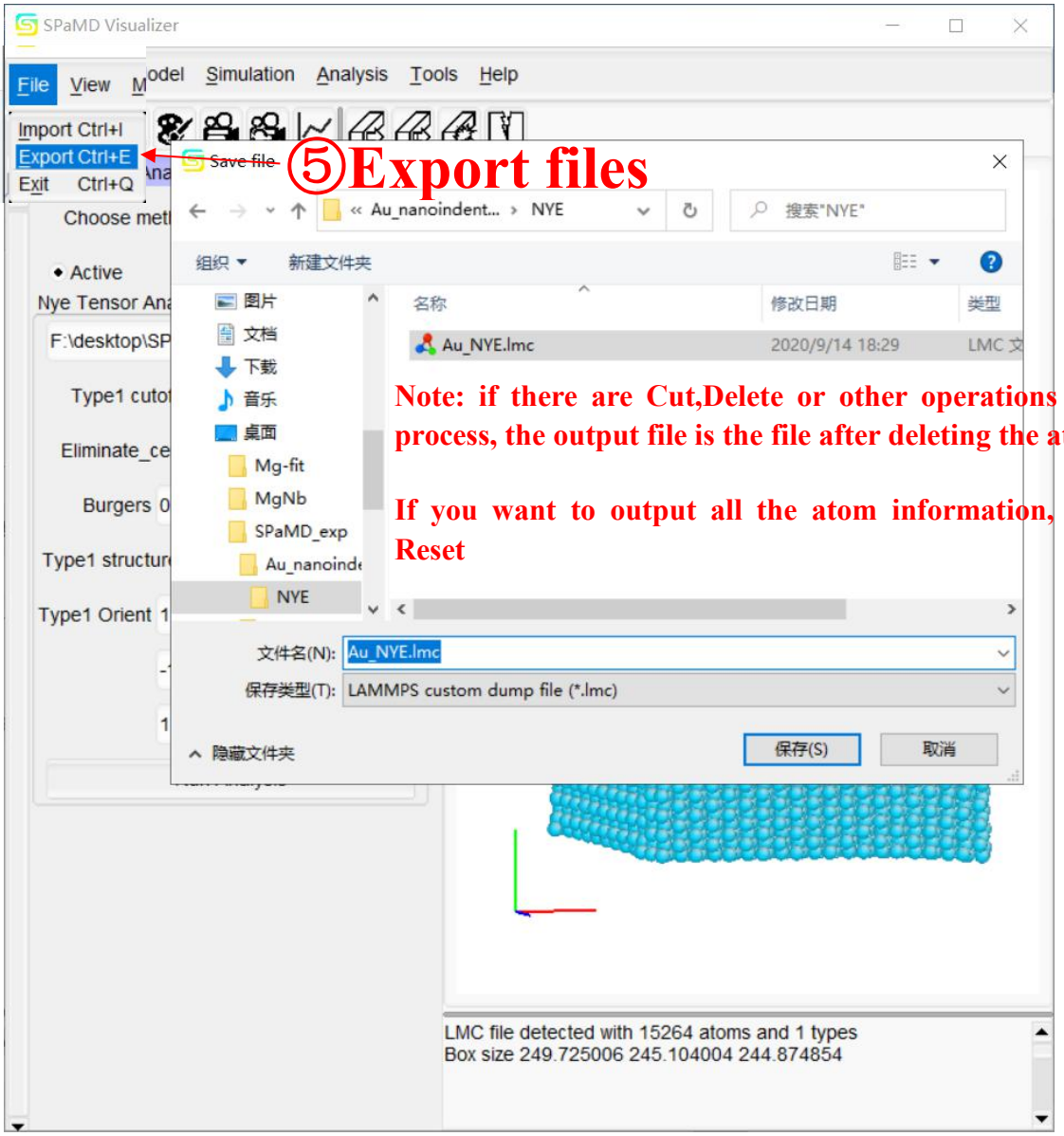
⑤ Click File Export to export files : Au_CNA.lmp




SPaMD Visualizer
File View Model Simulation Analysis Tools Help
View Model Analysis
Take CNA as an example
Choose method: cna
Active
Adaptive
Manual
Type1 cutoff Min 0
Max 0
②Select the mode of analysis and activate
The model read in is displayed here indicating that ① is completed successfully


SPaMD Visualizer
File View Model Simulation Analysis Tools Help
View Model Analysis
Choose method: cna
Active
Common Neighbor Analysis
Adaptive
Manual
Type1 cutoff Min 0
Max 0
Run Analysis
③Set the parameter and run analysis
Comparing with the figure above, it can be seen that CNA analysis has been completed.


SPaMD Visualizer
File View Model Simulation Analysis Tools Help
④View
View Model Analysis
Choose control: Setting
Color Coding:
Color Bar
Coloring
Input: cna Min .66664 Max .66664
RGB Bar
Color difference range
R: type G: type B: type
Trimming:
Normal X: 1
Normal Y: 0
Normal Z: 0
Distance: 100
Slice Width: 3
Trimming
Cut Recover
Show Slice Region
Show Slice Region
From: type Min 0 Max 1
Delete Recover
Inverse Reset
Atoms:
Other functions
Relative Radius: type1 1
LMC file detected with 15264 atoms and 1 types
Box size 249.725006 245.104004 244.874854



Note: if there are Cut,Delete or other operations in the view process, the output file is the file after deleting the atom

If you want to output all the atom information, please click Reset

3.1.2 STA Analysis

Main Process：

① Read file

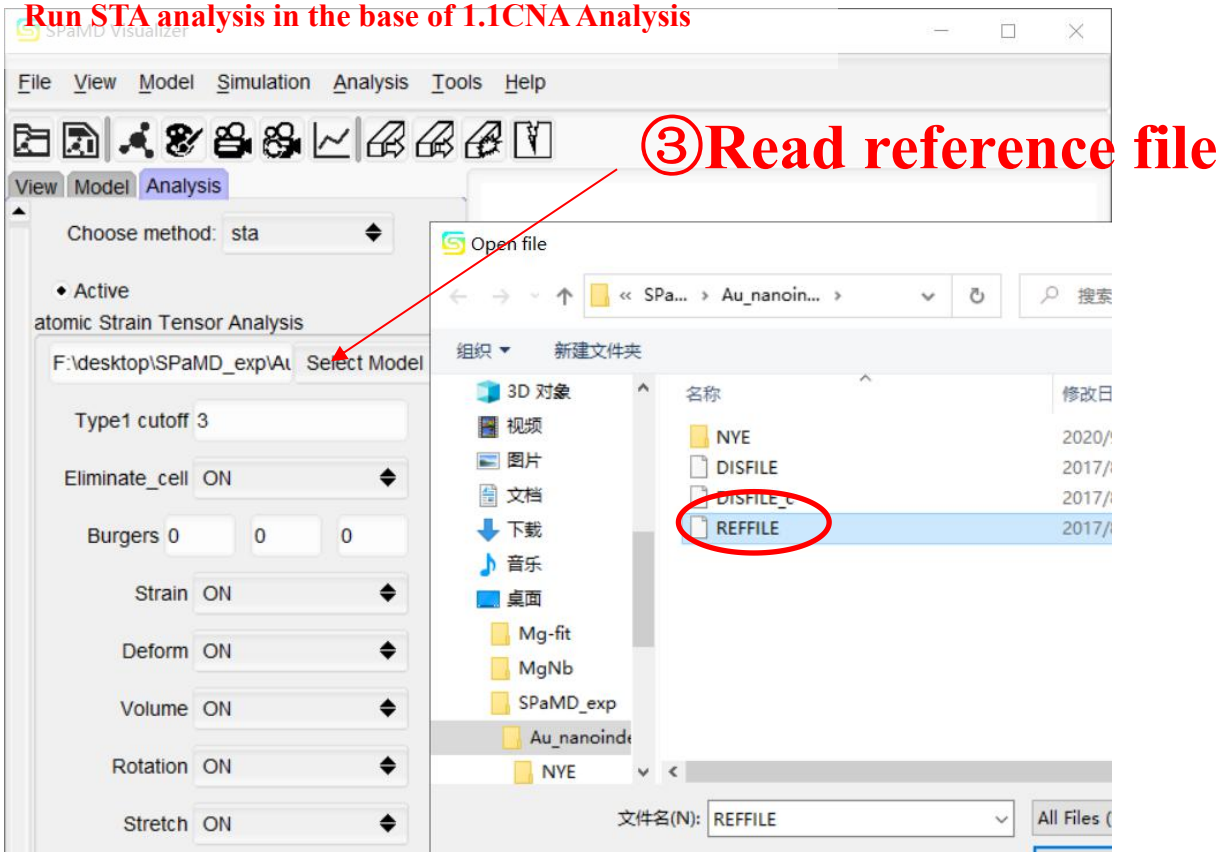
② Select the method of research:STA and activate_Active

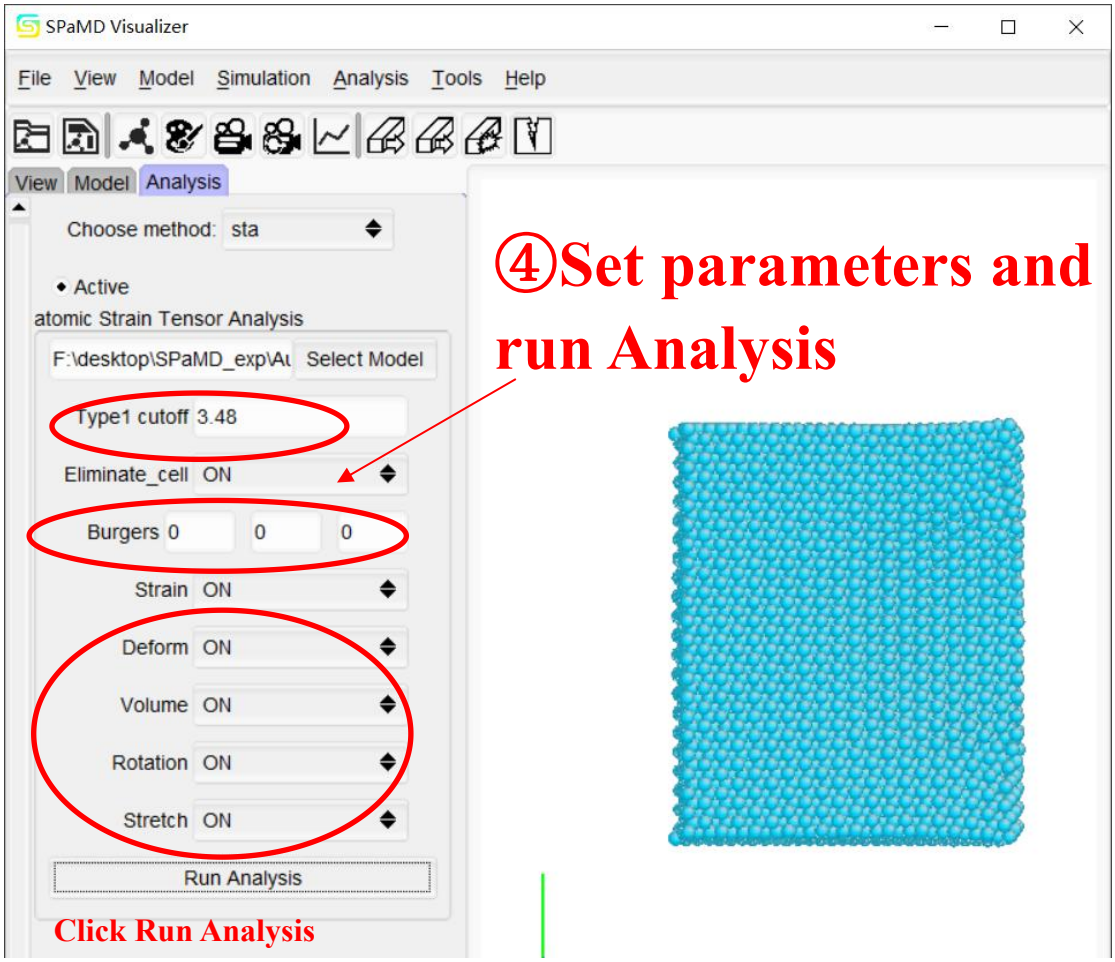
③ Select the reference file_REFILE

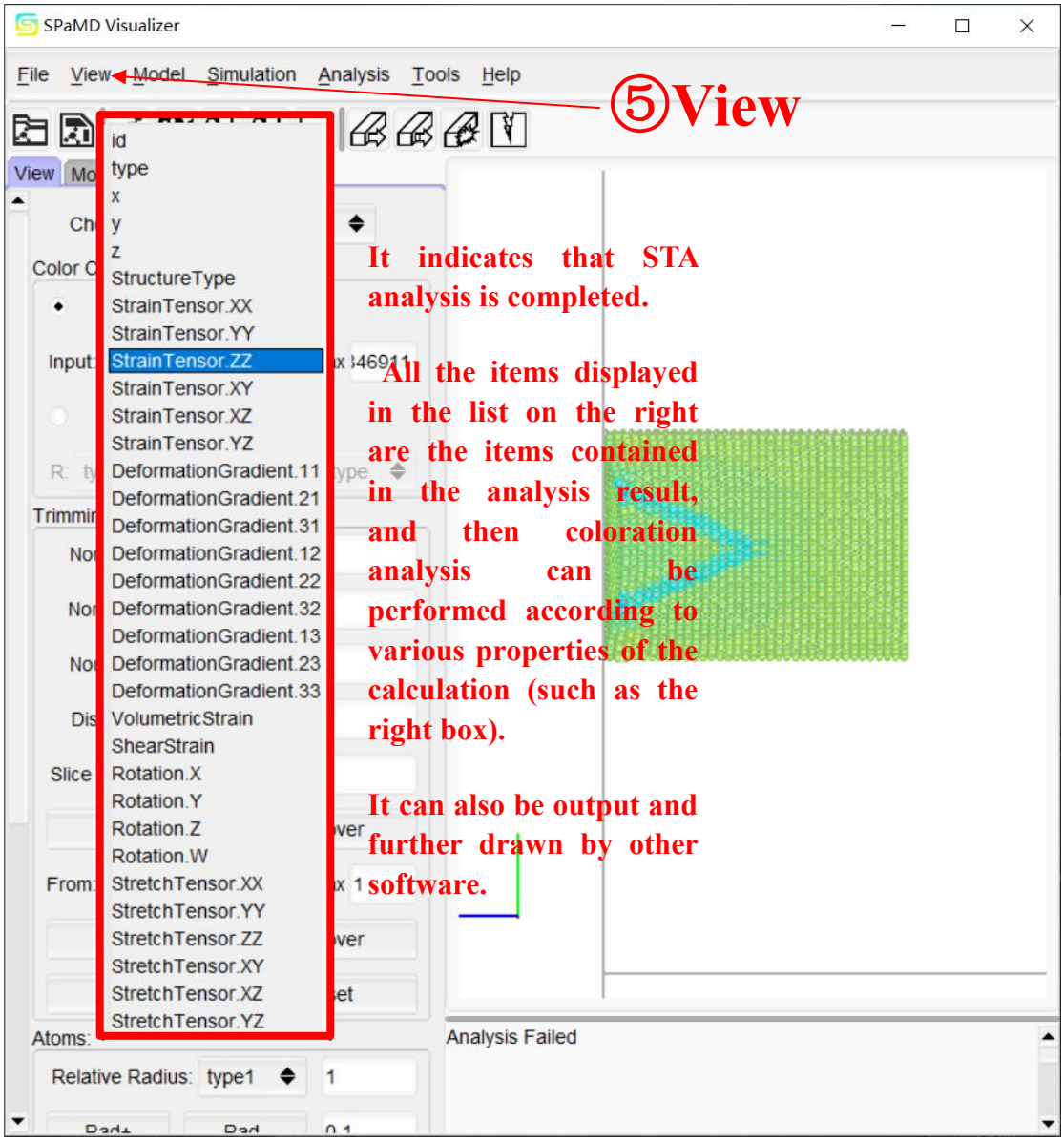
④ Set a series of parameters and click Run Analysis

⑤ Use View for visual viewing

⑥ File Export　: Au_STA.lmp




SPaMD Visualizer
File View Model Simulation Analysis Tools Help
View Model Analysis
Choose method: sta
Active
atomic Strain Tensor Analysis
F:\desktop\SPaMD_exp\Au
Select Model
Type1 cutoff 3.48
Eliminate_cell ON
Burgers 0 0 0
Strain ON
Deform ON
Volume ON
Rotation ON
Stretch ON
Run Analysis
Click Run Analysis
④Set parameters and run Analysis



Files Export

Output a file containing various properties of the calculation_ Au_ STA.lmc

This file contains all the calculation information in the red box above. Later, we can use Originpro, MATLAB and other software to further process and plot the data.

3.1.3 SVA Analysis

Main Process：

① Read file

② Select the method of research :SVA and activate_Active

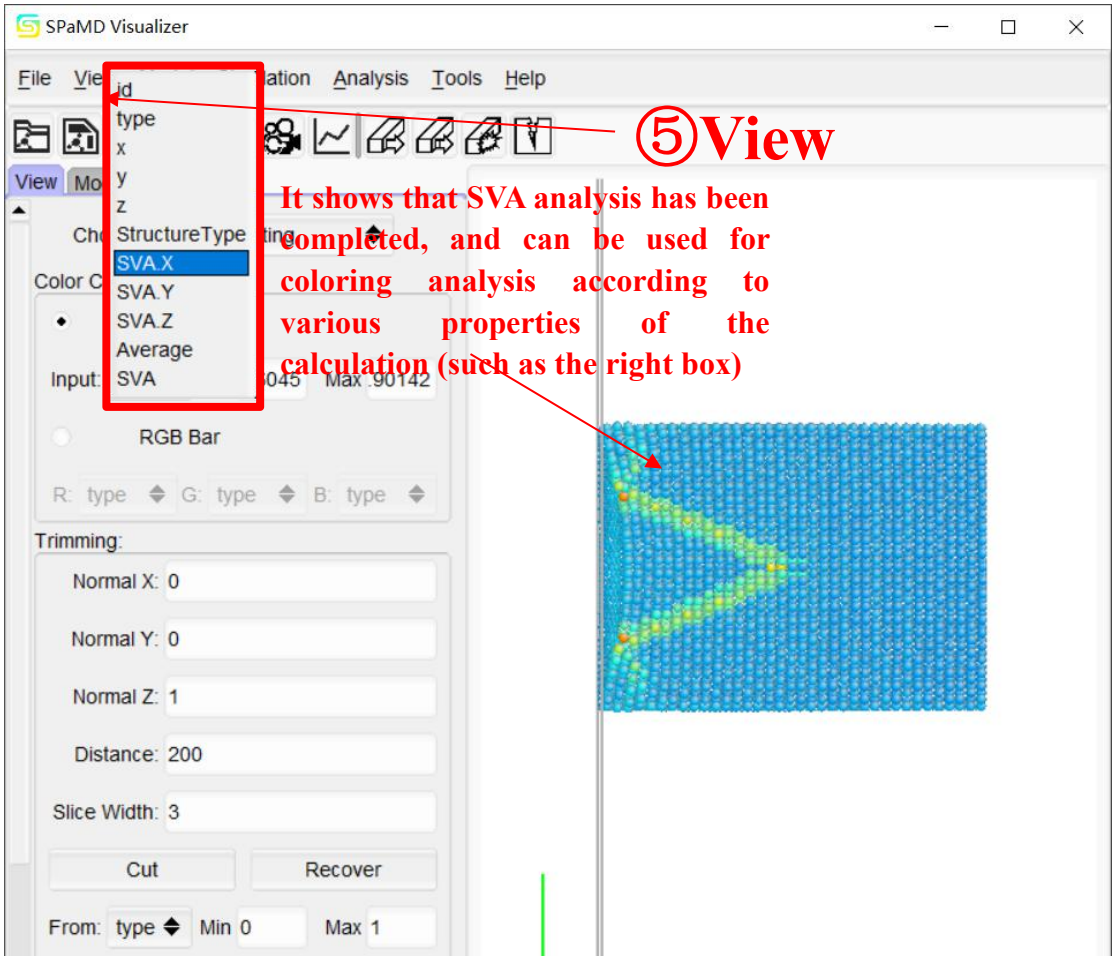
③ Select the reference file_REFILE

④ Set a series of parameters and click Run Analysis

⑤ Use View for visual viewing

⑥ File Export : Au_SVA.lmp

No more details for ①②③④



Files Export

Output a file containing various properties of the calculation_ Au_ STA.lmc.

Later, we can use originpro, MATLAB and other software for further drawing.

3.1.4 NTA Analysis

Main Process：

① Read file

② Select the method of research : NTA and activate_Active

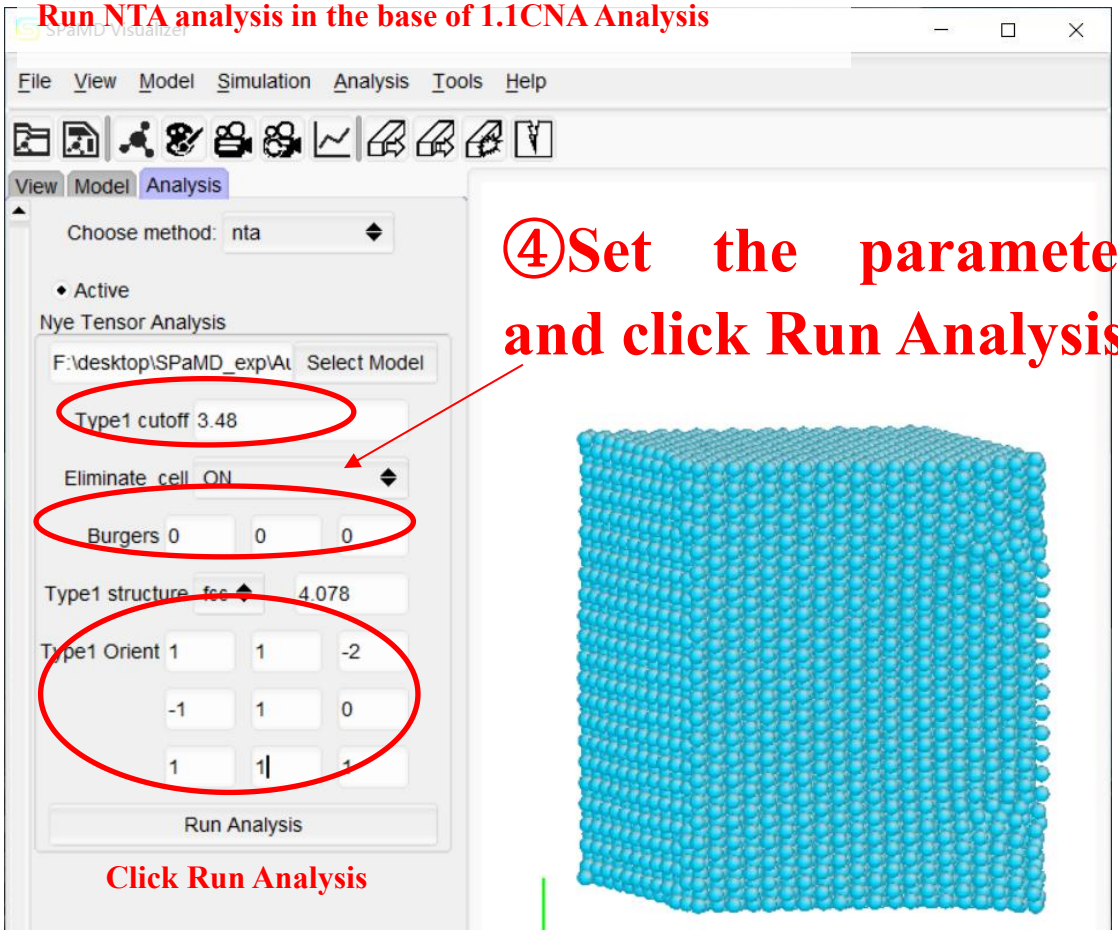
③ Select the reference file_REFILE

④ Set a series of parameters and click Run Analysis

⑤ Use View for visual viewing

⑥ File Export : Au_NTA.lmc。

No more details for ①②③⑤



⑦ Files Export

For the output Au_NTA.lmc,use other professional drawing software, such as originpro, MATLAB, for further drawing.

3.2 CuNi mismatch dislocation

3.2.1 CNA Analysis

Main Process：

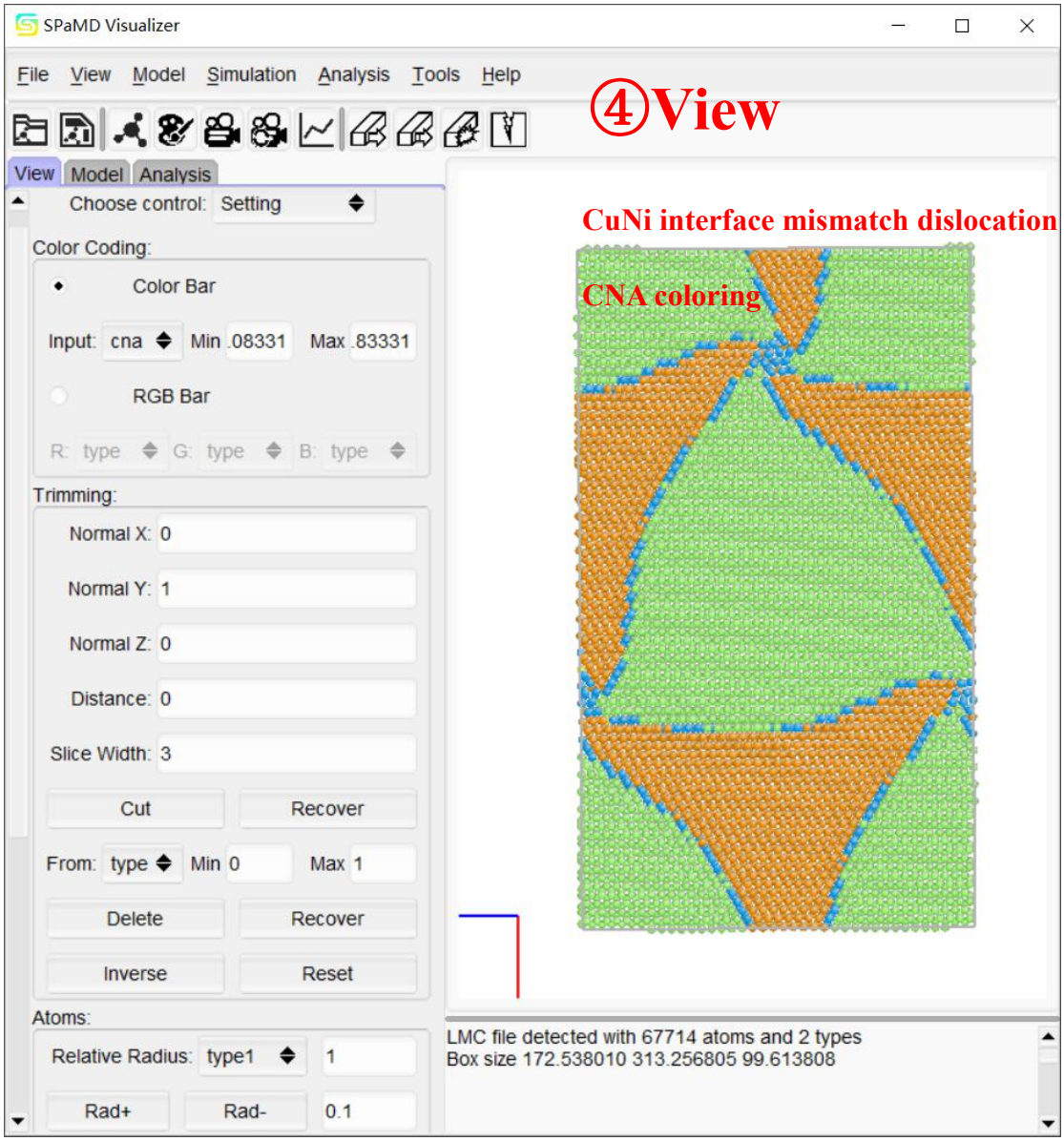
① Read file

② Select the method of research_CNA and activate_Active

③ Set a series of parameters and click Run Analysis

④ Use View for visual viewing

⑤ File Export ： CuNi_CNA.lmc



3.2.2 IDA Analysis

Main Process：

① Read file

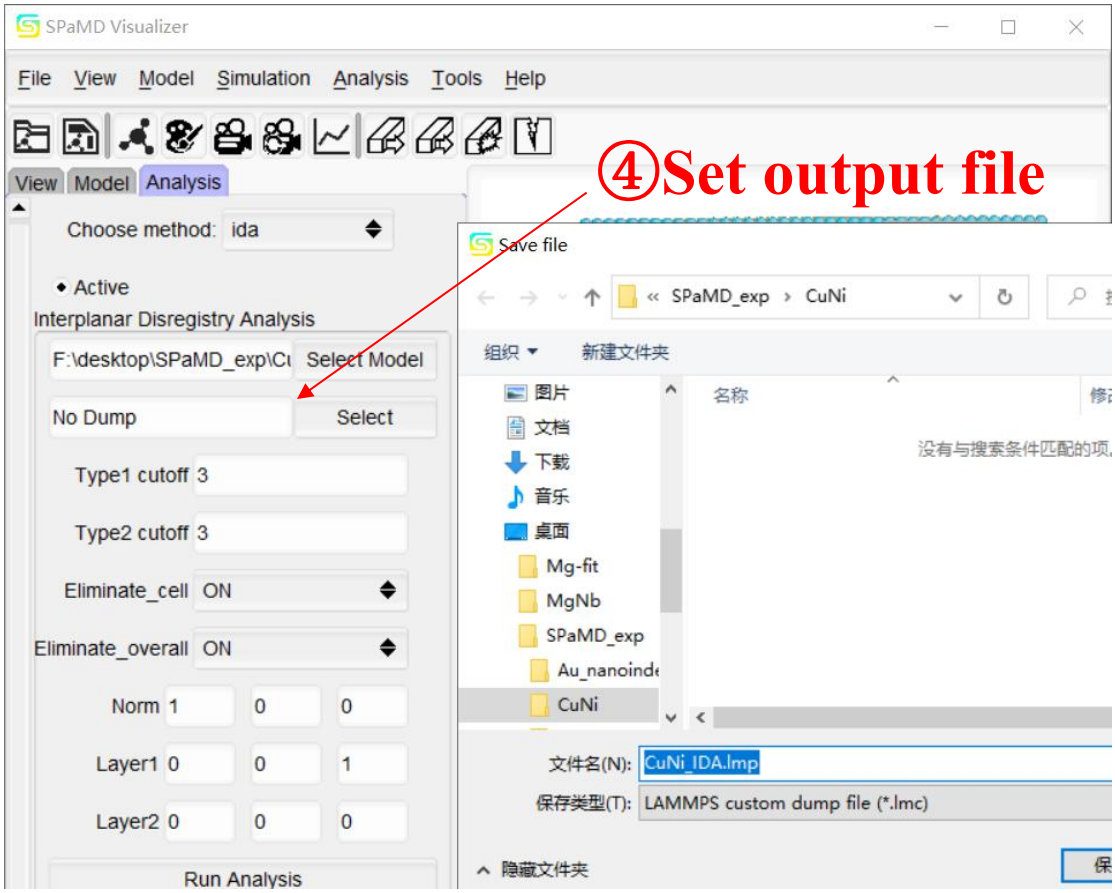
② Select the method of research: IDA and activate_Active

③ Select the reference file_REFILE

④ Specify the path and name of the output file _CuNi_IDA.lmc

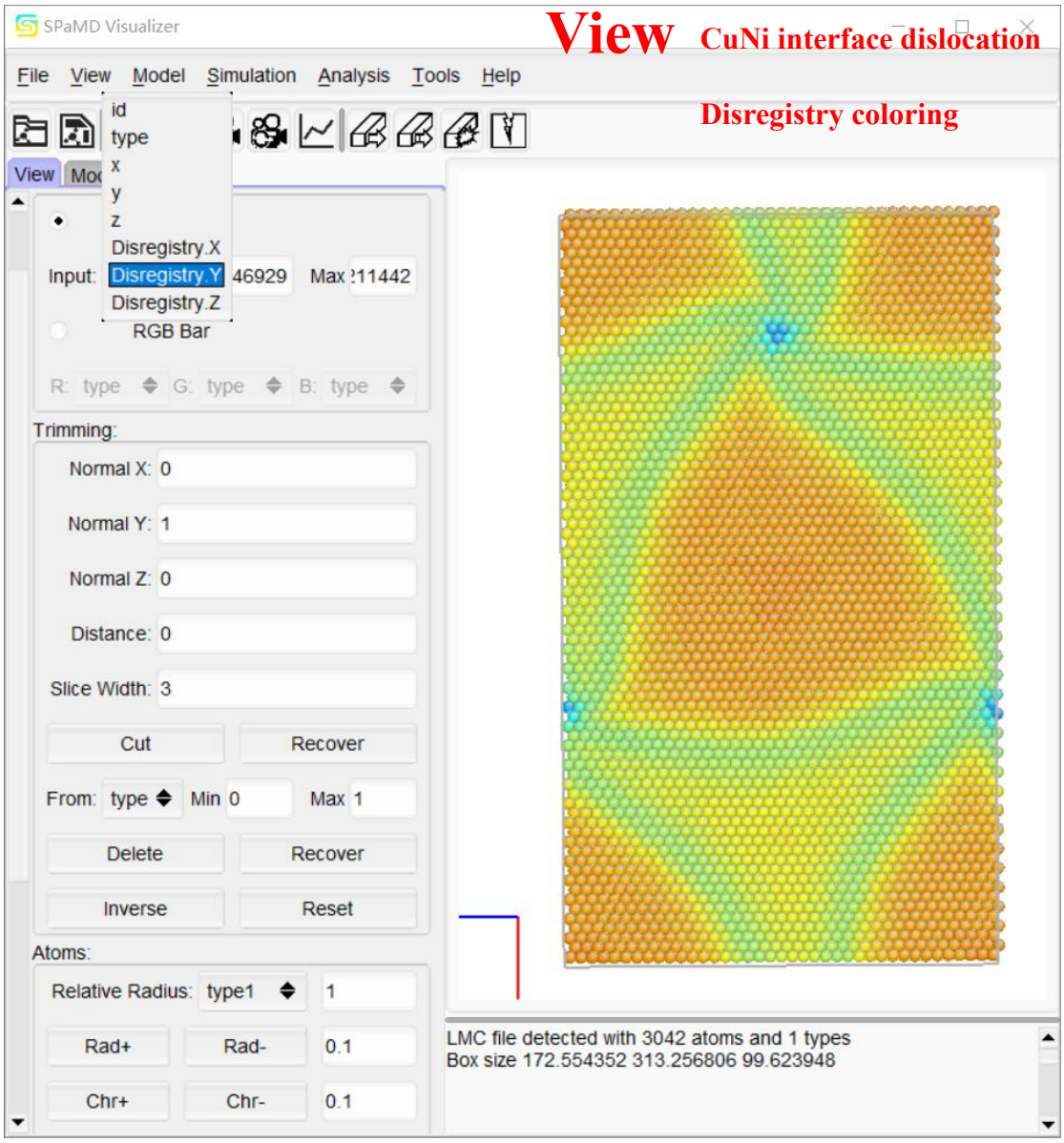
⑤ Set a series of parameters and click Run Analysis

⑥ Read CuNi_IDA.lmc file again and Use View for visual viewing



Note: for the atomic number of the result obtained by this analysis method is different from that of the initial model file, you need to specify the output name and path before analysis.

After analysis is completed, you need to open the output file before further observation.



3.2.3 NTA Analysis

Main Process：

① Read file

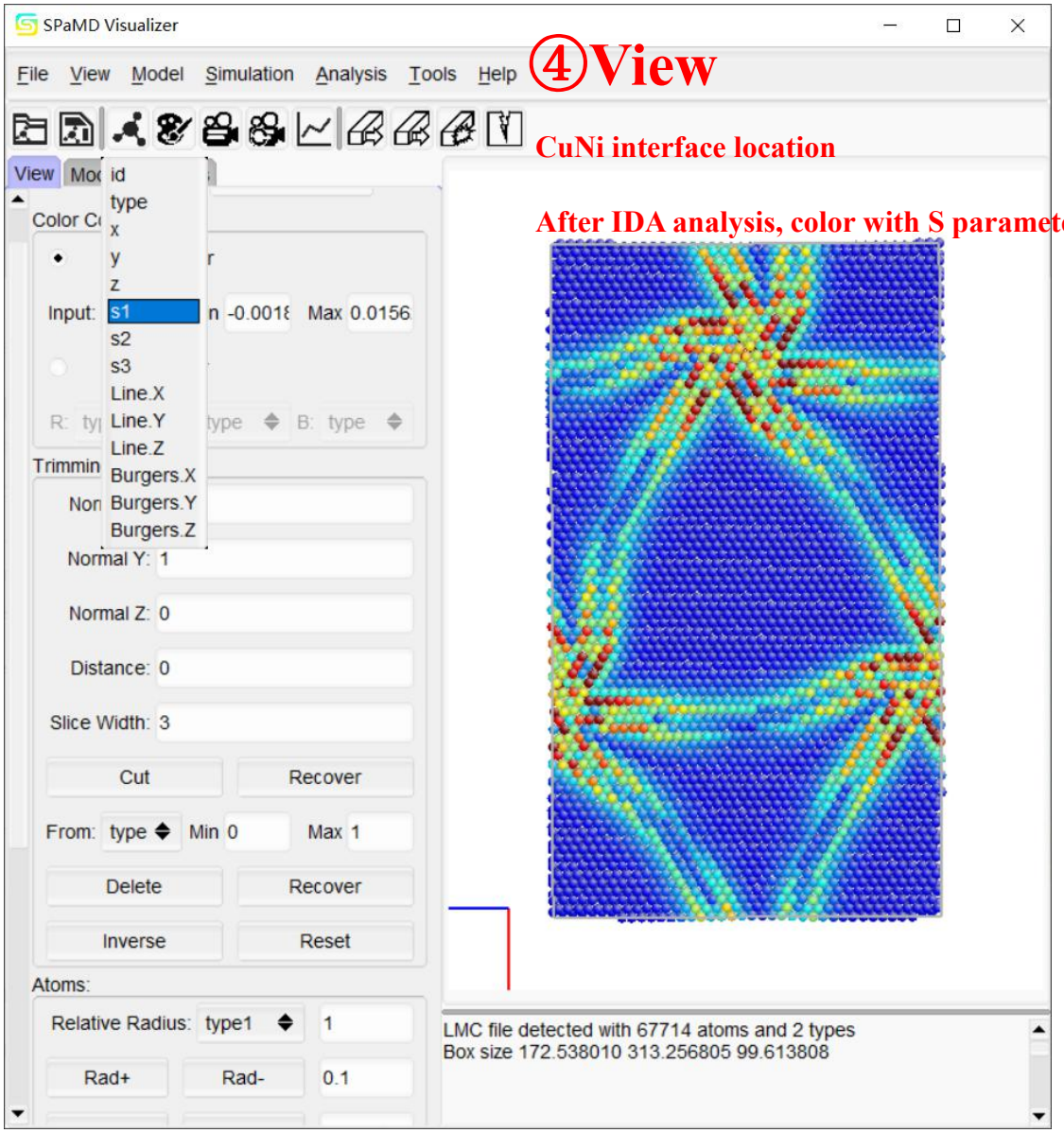
② Select the method of research :NTA and activate_Active

③ Select the reference file_REFILE

④ Set a series of parameters and click Run Analysis

⑤ Use View for visual viewing

⑥ File Export : CuNi_misfit_NTA.lmc



3.3 Tensile nucleation of CuNi

3.3.1 CNA Analysis

Main Process：

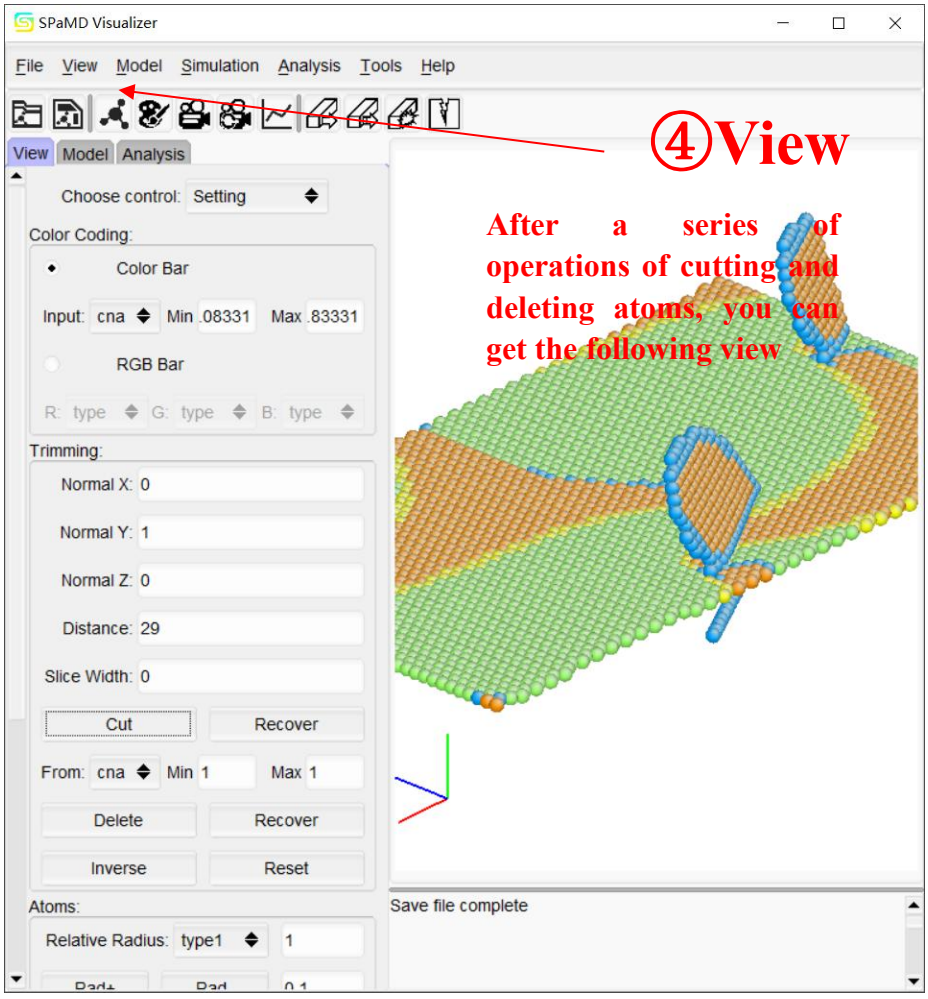
① Read file

② Select the method of research :CNA and activate_Active

③ Set a series of parameters and click Run Analysis

④ Use View for visual viewing

⑤ File Export : CuNi_tensile_CNA.lmp



⑥ **Files Export**

Note: the output file is the file after cutting and deleting atoms, which is convenient for further drawing

To output all atomic information files, click Reset to clear all operations before output

3.3.2 IDA Analysis

Main Process：

① Read file

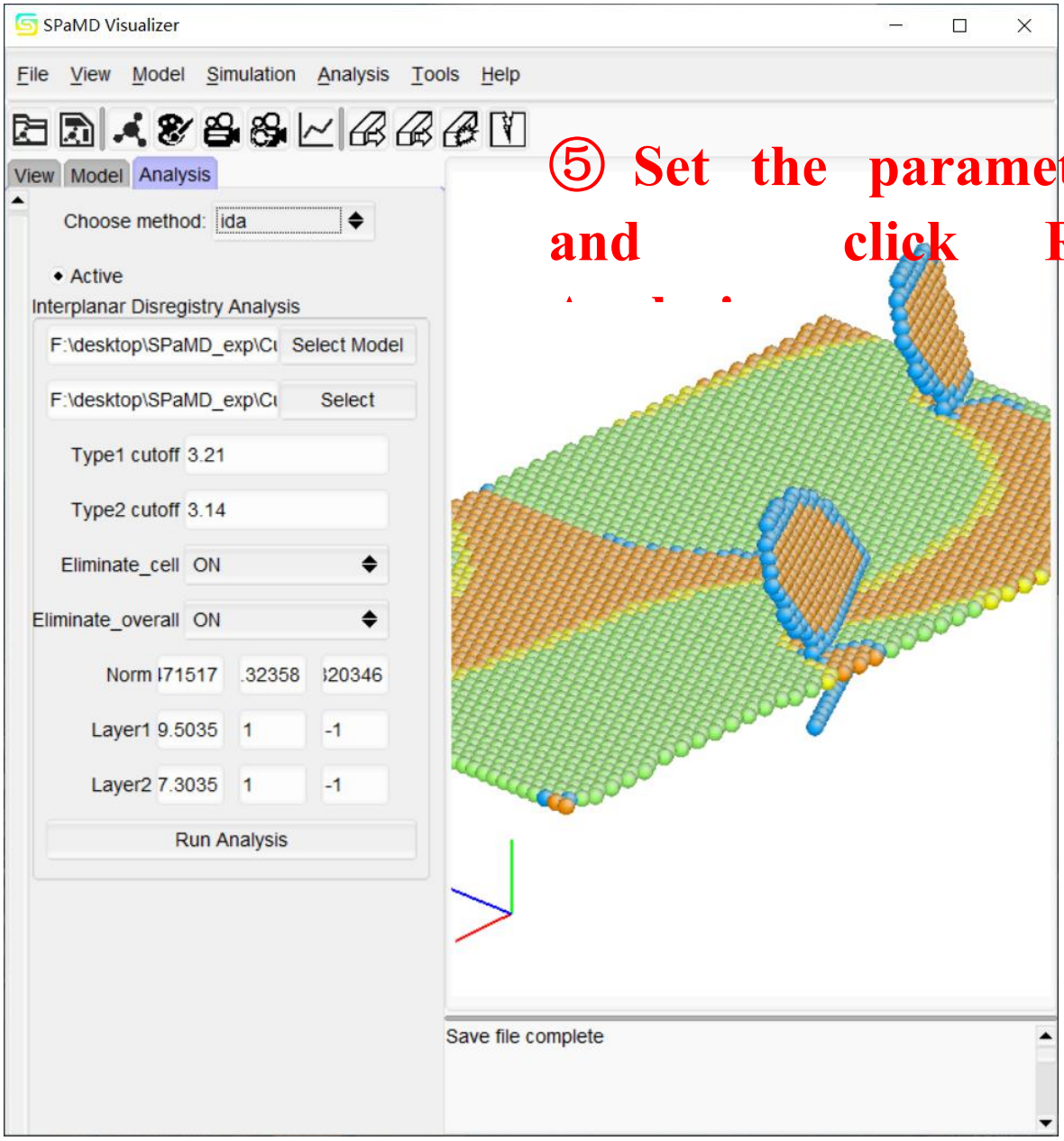
② Select the method of research:IDA and activate_Active

③ Select the reference file_REFILE

④ Specify the path and name of the output file : CuNi_IDA.lmc

⑤ Set a series of parameters and click Run Analysis

⑥ Read CuNi_tensile_IDA.lmc file again. Use View for visual viewing



3.4 Fe_screw dislocation

3.4.1 NTA Analysis

Main Process：

① Read file

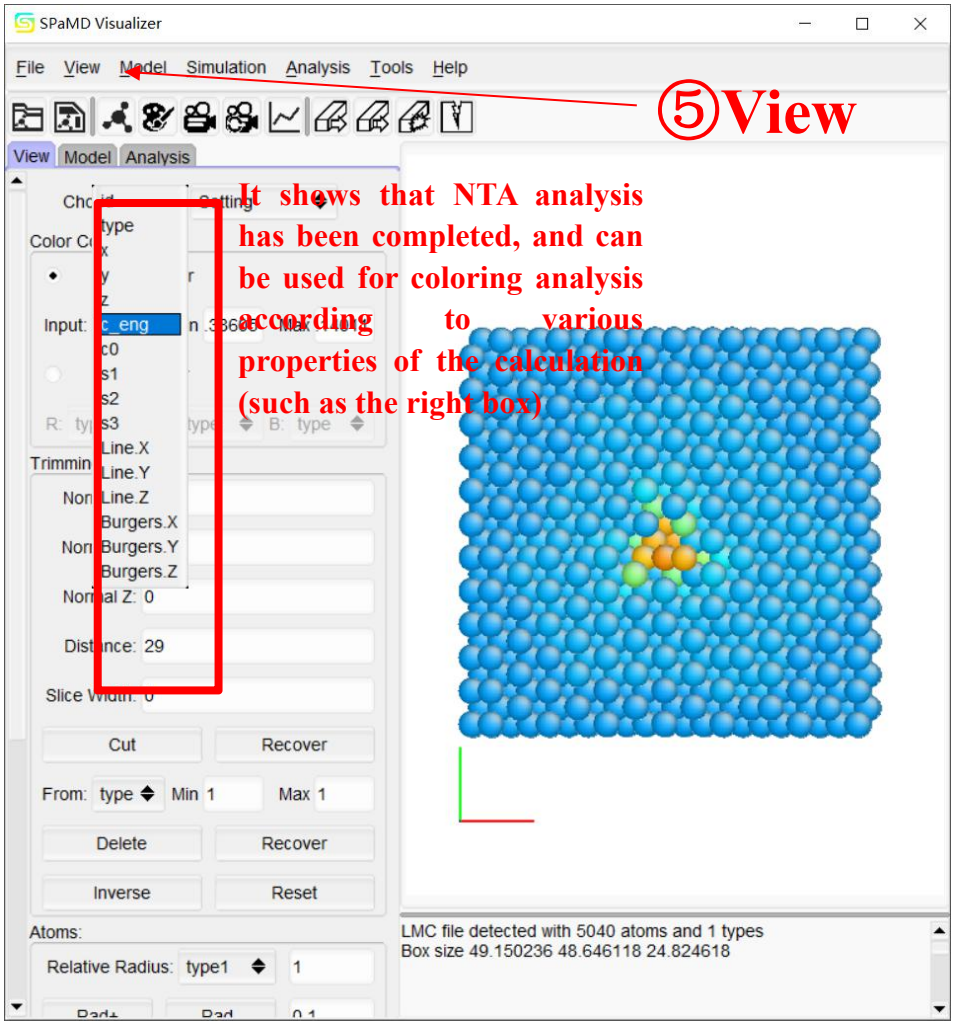
② Select the method of research : NTA and activate_Active

③ Select the reference file_REFILE

④ Set a series of parameters and click Run Analysis

⑤ Use View for visual viewing

⑥ File Export : Mg_NTA.lmc



⑦ **Files Export**

Output a file containing various properties of the calculation_ Au_ Nta_lmc, later users can use originpro, MATLAB and other software for further drawing

3.4.2 DDA Analysis

Main Process：

① Read file

② Select the method of research :DDA and activate_Active

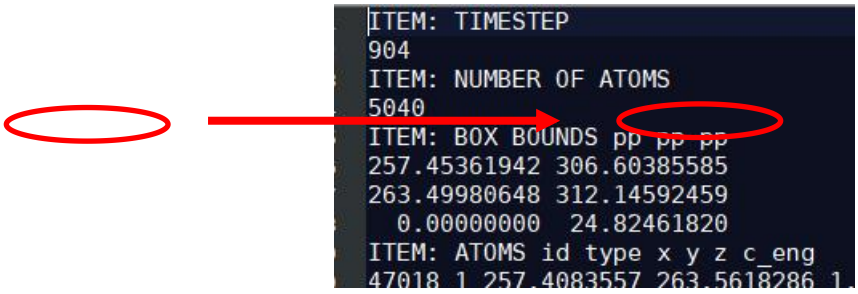
③ Select the reference file_REFILE

④ Specify the path and name of the output file: Fe_DDA.lmc

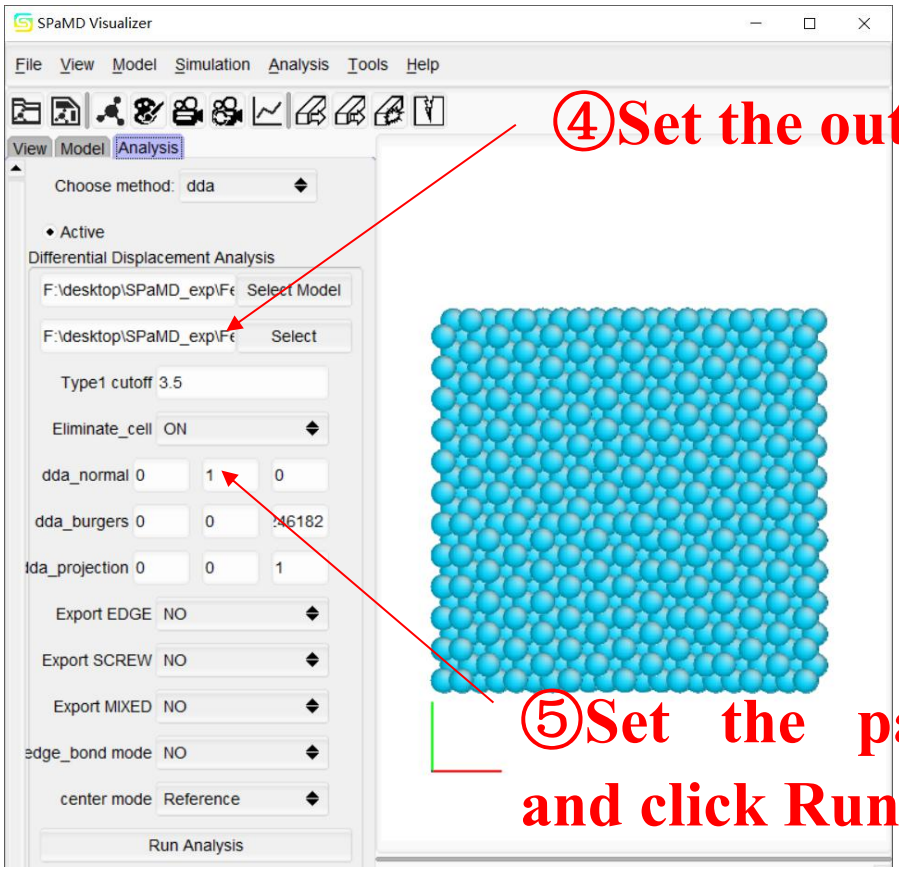
⑤ Set a series of parameters and click Run Analysis

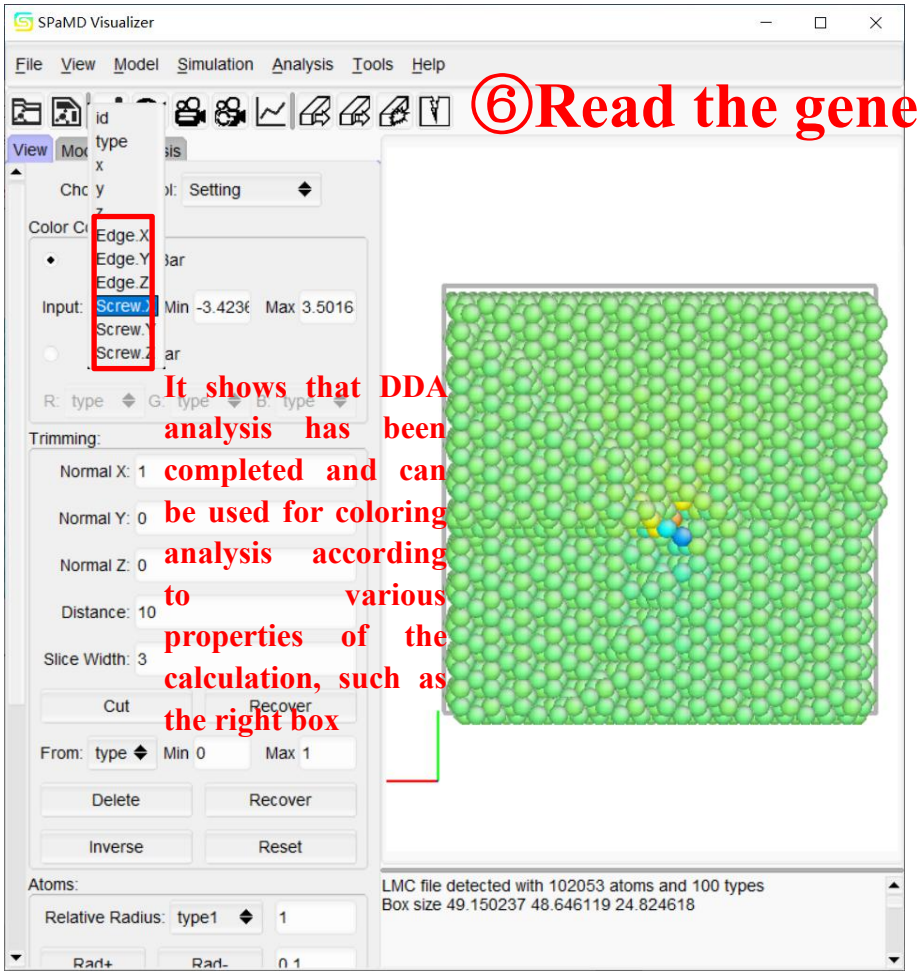
⑥ Read Fe_DDA.lmc file again. Use View for visual viewing

Note: because the periodicity of the read model file is p, and the periodicity requirement of the aadis program is s s p, but the function of periodicity is not involved in the SPaMD at present, so it is necessary to modify the periodicity of the model file manually




```
1  ITEM: TIMESTEP
2  904
3  ITEM: NUMBER OF ATOMS
4  5040
5  ITEM: BOX BOUNDS ss ss pp
6  257.45361942 306.60385585
7  263.49980648 312.14592459
8    0.00000000  24.82461820
9  ITEM: ATOMS id type x y z c_eng
10 47018 1 257.4083557 263.5618286
```


SPaMD Visualizer
File View Model Simulation Analysis Tools Help
View Model Analysis
Choose method: dda
Active
Differential Displacement Analysis
Select Model
Select
Type1 cutoff 3.5
Eliminate_cell ON
dda_normal 0 1 0
dda_burgers 0 0
dda_projection 0 0 1
Export EDGE NO
Export SCREW NO
Export MIXED NO
edge_bond mode NO
center mode Reference
Run Analysis
④Set the output
⑤Set the parameters and click Run Analysis


SPaMD Visualizer
File View Model Simulation Analysis Tools Help
id
type
x
y
Edge.X
Edge.Y
Edge.Z
Screw.X
Screw.Y
Screw.Z
Setting
Input:
Min -3.4236
Max 3.5016
Trimming:
Normal X: 1
Normal Y: 0
Normal Z: 0
Distance: 10
Slice Width: 3
Cut
Recover
From: type
Min 0
Max 1
Delete
Recover
Inverse
Reset
Atoms:
Relative Radius: type1 1
LMC file detected with 102053 atoms and 100 types
Box size 49.150237 48.646119 24.824618
⑥Read the generated file
It shows that DDA analysis has been completed and can be used for coloring analysis according to various properties of the calculation, such as the right box

3.5 Fe Grain boundary torsion

3.5.1 CNA Analysis

Main Process：

① Read file

② Select the method of research_CNA and activate_Active

③ Set a series of parameters and click Run Analysis

④ Use View for visual viewing

⑤ File Export : Fe_CNA.lmp

3.5.2 NYE Analysis

Main Process：

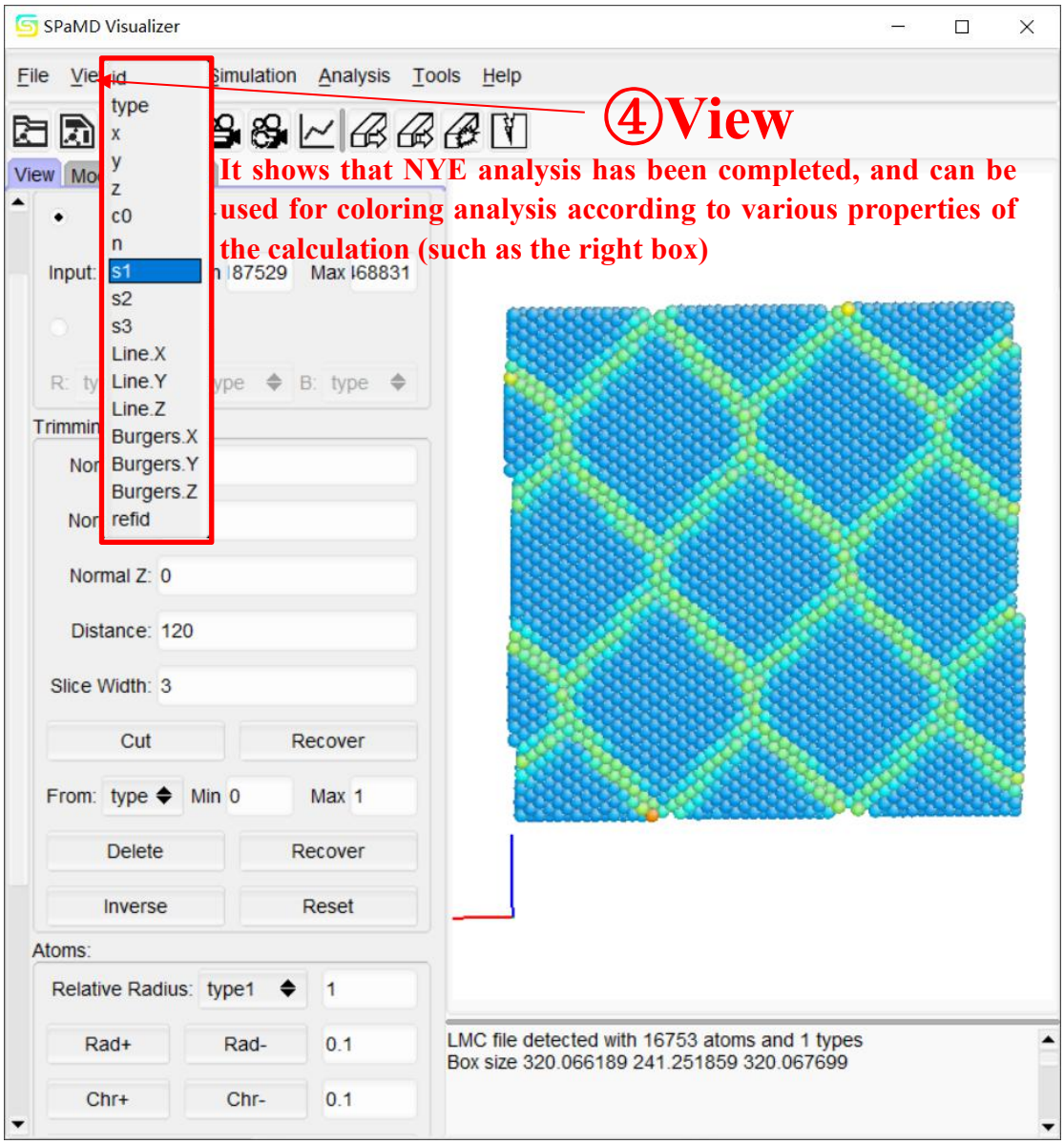
① Read file

② Select the method of research :NYE and activate_Active

③ Set a series of parameters and click Run Analysis

④ Use View for visual viewing

⑤ File Export : Fe_twist_Nye.lmc

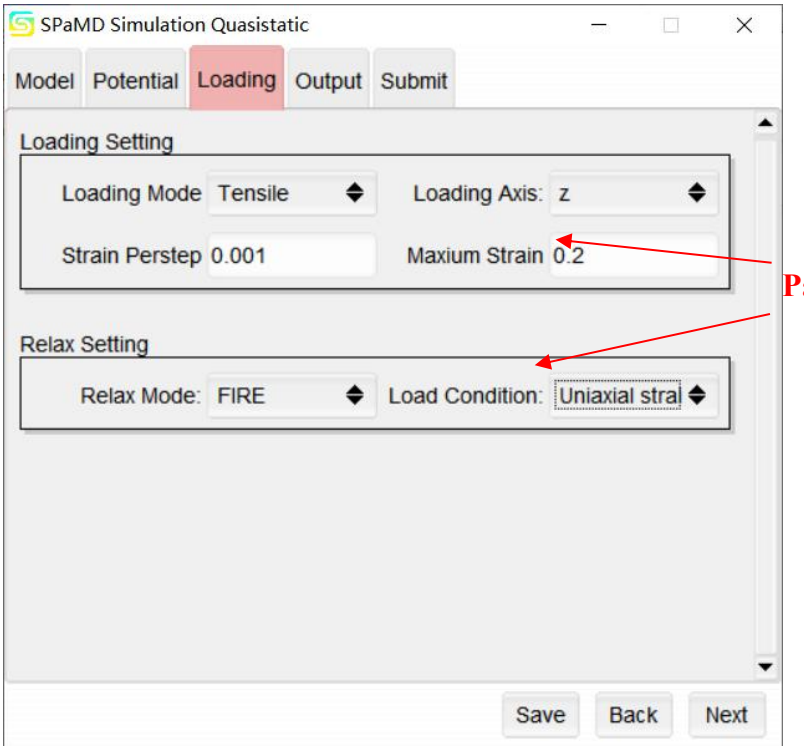


Appendix

（Note: the contents in the appendix are the functions of the simulation module. The following shows some functions and simulation results, which are not yet open. ）

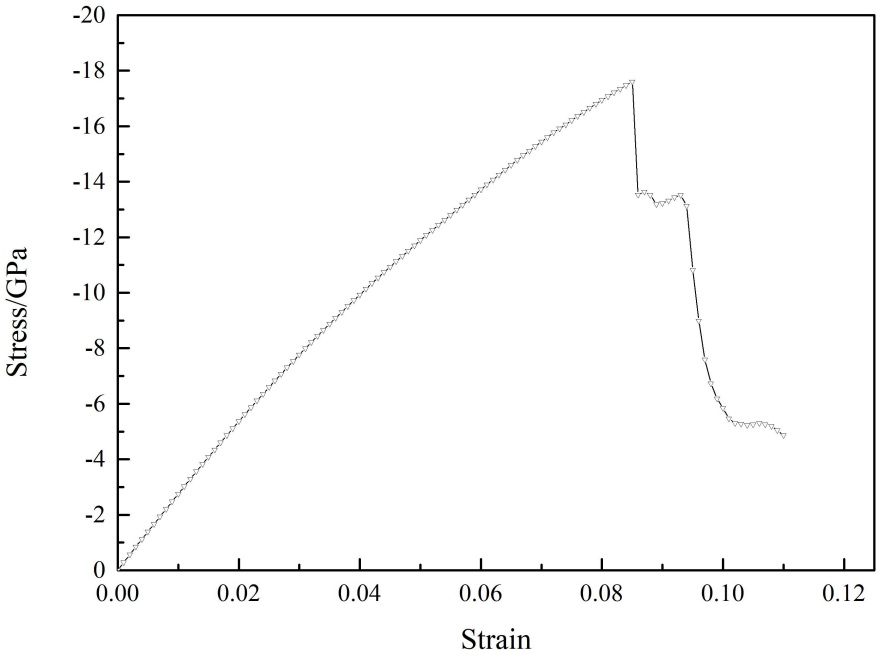
1. Quasistatic

• Parameter setting: loading mode, loading direction, strain gradient and relaxation mode

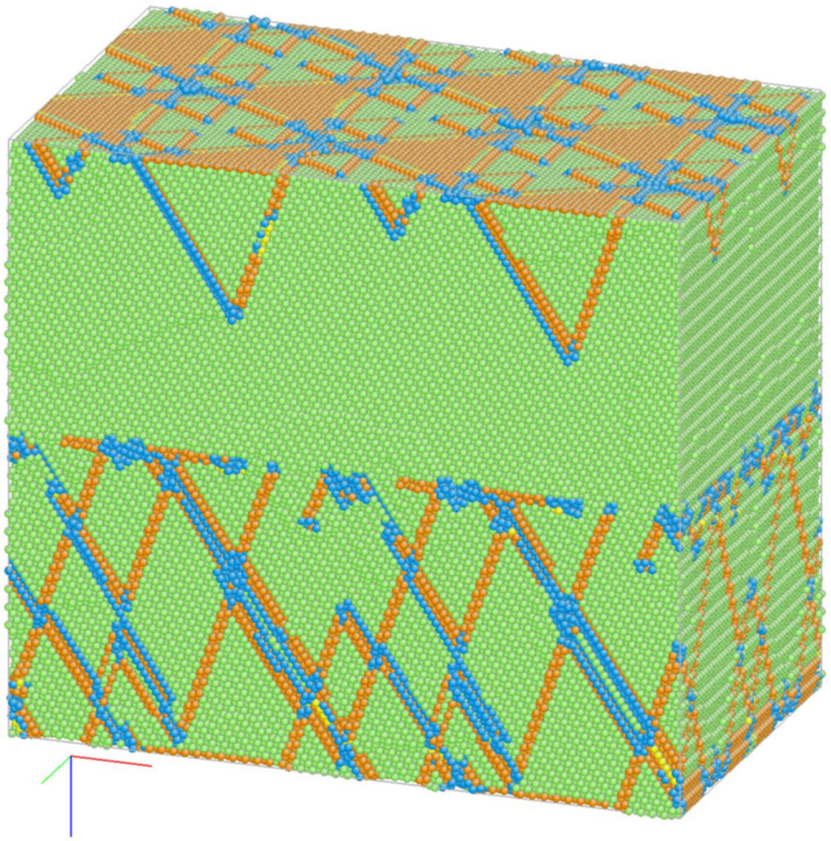


Parameter setting

•The stress-strain curve is drawn after loading:

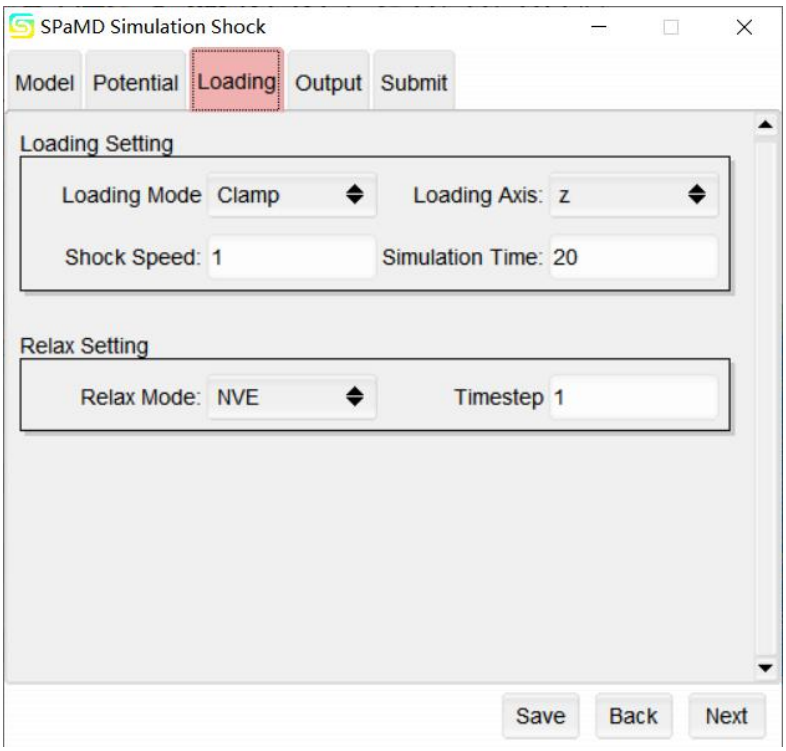


•Loaded model:

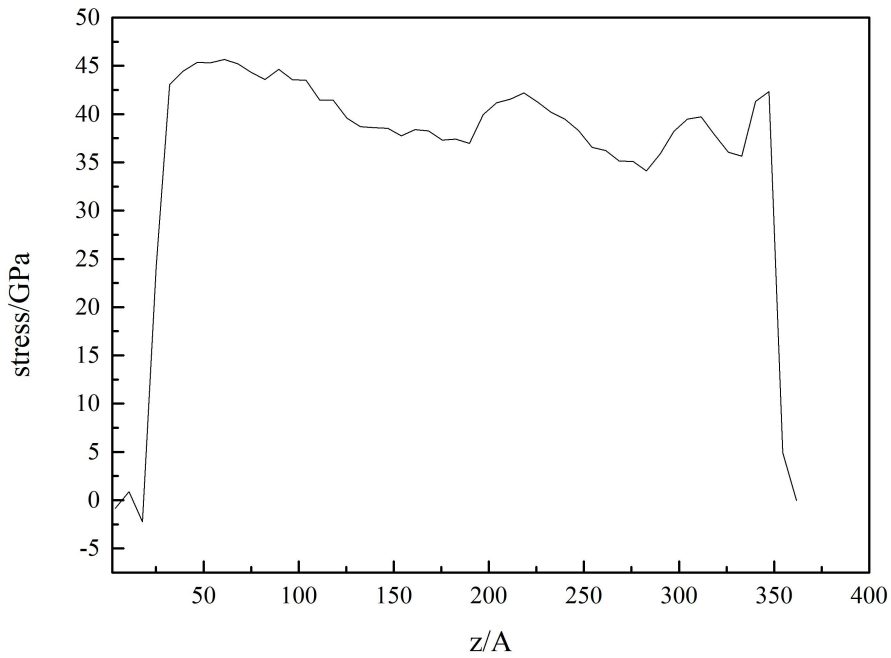


2. Shock

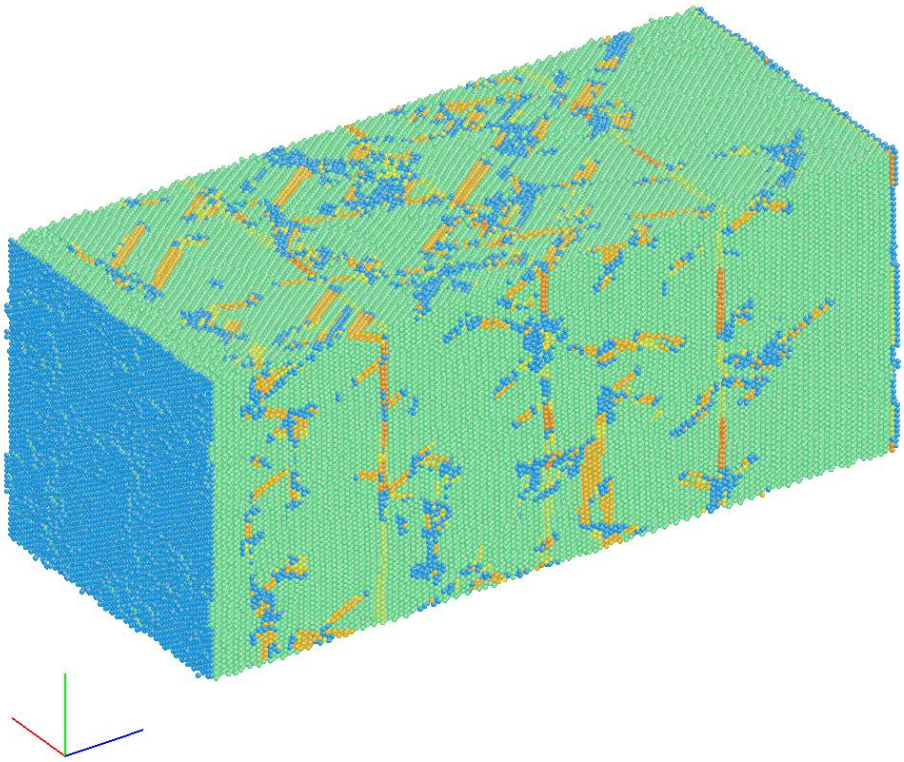
- Parameter setting:



- Stress strain curve:

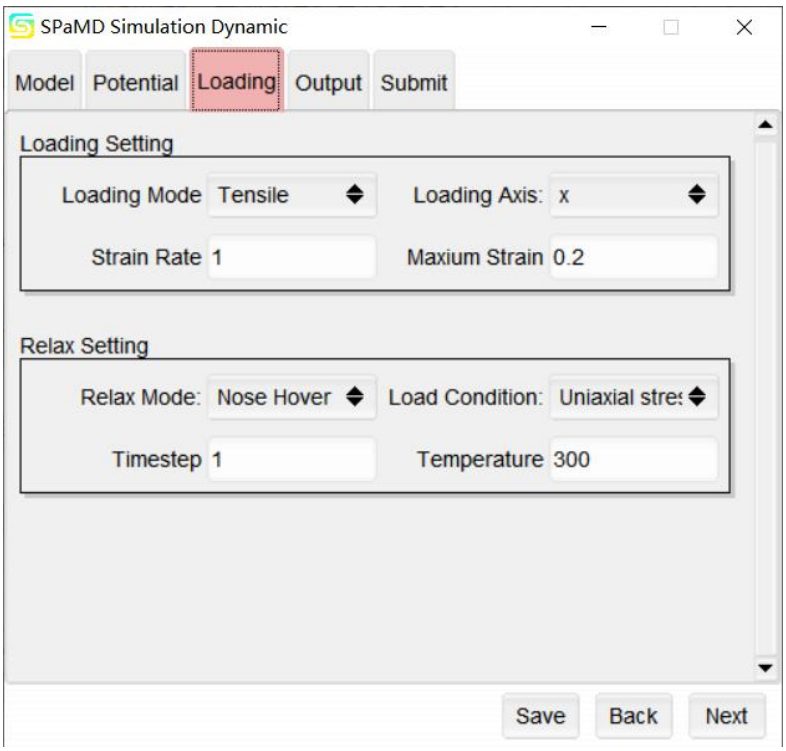


- Loaded model:

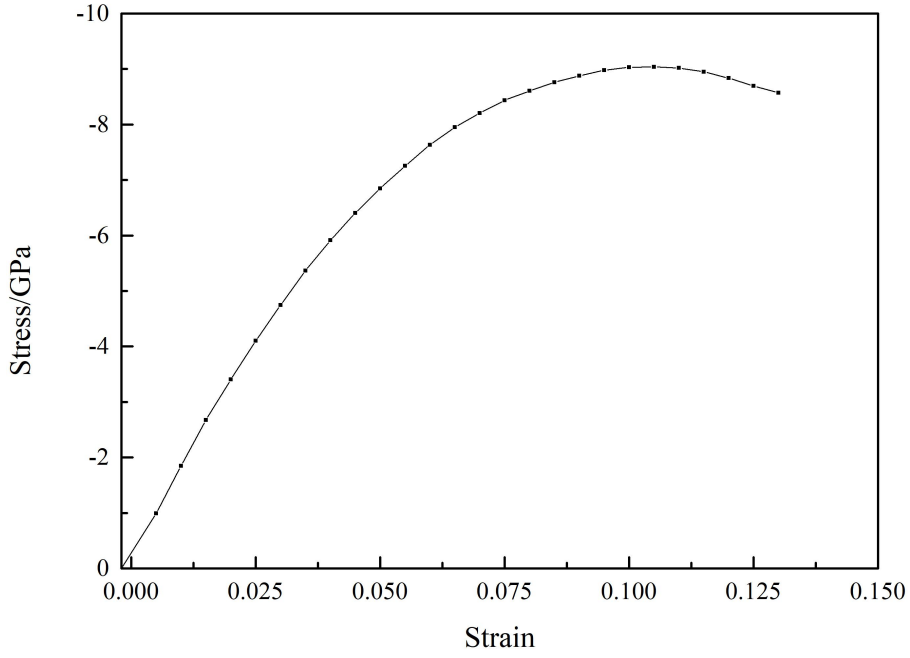


3. Dynamic

- Parameter setting:



- Stress strain curve:



- Loaded model: