

Multislice for TEM

The original DOS programs were developed by Dr. Earl J. Kirkland and distributed with "Advanced Computing in ELECTRON MICROSCOPY" published by Plenum Press (1998).

This Windows software was made by referring to and rewriting them so as to be easy to use.

It is strongly recommended that you should purchase the book and understand the details of the theory.

Chapter I: Conventional TEM Image

\$1. General procedures for simulating a conventional TEM image

- 1) Make input data files (wwwi.dat) for the atomic potentials of a specimen.

Note: Usually, $i = a, b, c, \dots$

- 2) Execute "Atomic Potential" function by using the each input data file (wwwi.dat) $\langle i = a, b, c, \dots \rangle$, and get atomic potential files (wwwipot.tif) $\langle i = a, b, c, \dots \rangle$.
- 3) Execute "Multislice" function by using the atomic potential files (wwwipot.tif) $\langle i = a, b, c, \dots \rangle$, and get a multislice file (wwwmul.tif).
- 4) Execute "Image" function by using the multislice file (wwwmul.tif), and get an image file (wwwimg.tif).

\$2. Format of input data file for the atomic potential

The input data files for the atomic potential must have following format.

ax	by	cz	
Ns			
Sxa(1)	Sxb(1)	Sya(1)	Syb(1)
Sxa(2)	Sxb(2)	Sya(2)	Syb(2)
....
Sxa(Ns)	Sxb(Ns)	Sya(Ns)	Syb(Ns)
<one blank line>			
Z(atom-1)			
Occ(1)	xpos(1)	ypos(1)	wobble(1)
....
Occ(n1)	xpos(n1)	ypos(n1)	wobble(n1)
<one blank line>			
Z(atom-2)			
Occ(1)	xpos(1)	ypos(1)	wobble(1)
....
Occ(n2)	xpos(n2)	ypos(n2)	wobble(n2)
<one blank line>			
....
....
Z(atom-j)			
Occ(1)	xpos(1)	ypos(1)	wobble(1)
...
Occ(nj)	xpos(nj)	ypos(nj)	wobble(nj)
<one blank line>			
<one blank line>			

Note:

- 1) Super cell group:

* ax and by are dimensions of super cell of one slice of the specimen in Angstroms. cz is slice thickness.

- 2) Symmetry operation group:

* Ns is the number of symmetry operation for each coordinates.

* The number of lines for the symmetry operation followed by Ns row must match to Ns.

Regarding the symmetry operation, refer to the original book published by Plenum Press.

* If Ns is zero, <one blank line> which is located in the end of the Ns group, is not required.

- 3) Atomic coordinates group:

* One or more atomic coordinates group(s) must exist.

* Z(atom-i) is the atomic number of the i-th atom on a sliced plane.

- * Occ(i) is the occupancy of the atom. The occupancy is typically one, but able to set to a fractional value (Refer to the original book published by Plenum Press.).
 - * xpos(i) and ypos(i) are reduced coordinates of the atom.
 - * wobble(i) is the root mean square (rms) random displacement in each direction, for simulating thermal phonons, in Angstroms. Typically wobble(i) is zero.
- If the wobble(i) is not used for the simulation, the wobble(i) is not required in the input data file.
- * Each atomic coordinate group must terminate with <one blank line> at the end of the group.

4) End of input data file:

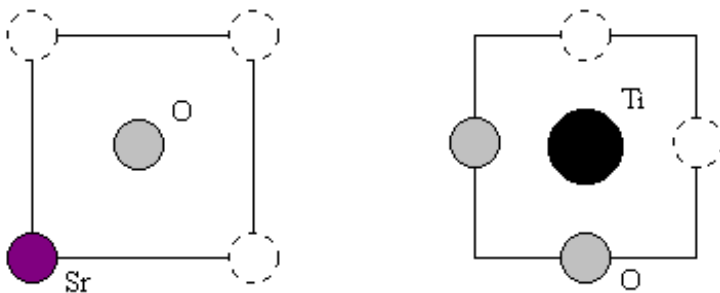
- * The end of input data file for the atomic potential must terminate with one blank line.
- In other words, two blank lines, including <one blank line> of the end of the atomic coordinates group, are required.

\$3. Example of input data file

The following examples of the atomic potential data simulate a conventional TEM image of strontium titanate (SrTiO₃) which has a cubic perovskite structure with a cubic unit cell of a=3.905 Angstroms.

Strontium (Sr) atoms are located in the all corners of the cubic. Oxygen (O) atoms are located in the center of each face of the cubic. Titanium (Ti) atom is located in the center of the cubic.

The “wobble(i)” are not applied and sliced planes are perpendicular to <001>.



The atomic potential input data file, SRTA.DAT, for the layer of Sr (Z=38) and O (Z=8), which is a face plane of the cube, is as follows;

```
3.905    3.905    1.9525
0
38
1.0      0.0      0.0
      ← one blank line
8
1.0      0.5      0.5
      ← one blank line
      ← one blank line
```

The atomic potential input data file, SRTB.DAT, for the layer of Ti (Z=22) and O (Z=8), which is a plane through the cube center parallel to the face plane, is as follows;

```
3.905    3.905    1.9525
0
22
1.0      0.5      0.5
      ← one blank line
8
1.0      0.5      0.0
1.0      0.0      0.5
      ← one blank line
      ← one blank line
```

\$3. Stacking sequence

- * When using “Multislice” function, it is required to input the "stacking sequence."
- * The stacking sequence is pair(s) of the slices of the specimen, and must be entered in p(xyz) form.
- * p is a positive integer which denotes the number of repeats of the sequence xyz (a pair of x, y, and z slices).
- * x, y and z are symbols of each slice, in the order abcd...xyzABCD...XYZ.

* The sequence xyz must be parenthesized.

For example, 12(ab) denotes twelve repeats of the sequence ab (a pair of a and b slices).

* The name of the first slice must be a, and the name of the second slice must be b, and so on, in the order abcd...xyzABCD...XYZ.

* Regarding the stacking sequence, parenthesis may be nested up to 100 levels and structures such as 5(2(ab)3(ca)) are allowed.

Chapter II: Convergent Beam TEM Image

\$1. General procedures for simulating a convergent beam TEM image

1) Make input a data file (www.xyz) for the autoslice calculation.

2) First, execute "Probe" function by using the input data file (www.xyz), and get a probe file (wwwprb.tif).

Note: When executing "Probe" function, the filename of a data file (www.xyz) is only referred.

3) Execute "Autoslice" function by using both of the data file (www.xyz) and the probe file (wwwprb.tif), and get an autoslice file (wwwmul.tif).

Note: It takes from several to several ten minutes to execute "Autoslice" function.

4) Execute "Image" function by using the autoslice file (wwwmul.tif), and get an image file (wwwimg.tif).

\$2. Format of input data file for the autoslice

The input data file for the autoslice must have following format.

One comment line

ax	by	cz			
Z(atom-1)	xpos(1)	ypos(1)	zpos(1)	Occ(1)	wobble(1)
Z(atom-2)	xpos(2)	ypos(2)	zpos(2)	Occ(2)	wobble(2)
Z(atom-3)	xpos(3)	ypos(3)	zpos(3)	Occ(3)	wobble(3)
....
....
Z(atom-j)	xpos(j)	ypos(j)	zpos(j)	Occ(j)	wobble(j)
-1					
Z(atom-1')	xpos(1')	ypos(1')	zpos(1')	Occ(1')	wobble(1')

Note:

1) Comment line:

* One line of comment is always required.

2) Unit cell dimension:

* ax, by and cz are dimensions of unit cell of a specimen in Angstroms.

3) Atomic coordinates group:

* One or more atomic coordinates line(s) must exist.

* Z(atom-i) is the atomic number of the atom on the i-th sliced plane.

* xpos(i), ypos(i) and zpos(i) are the X, Y, and Z positions of the atom on the i-th sliced plane in Angstroms respectively.

Note: These values must be actual values, not using reduced coordinate values.

* Occ(i) is the occupancy of the atom. The occupancy is typically one (1.0), but able to set to a fractional value (Refer to the original book published by Plenum Press.).

* wobble(i) is the root mean square (rms) random displacement, for simulating thermal phonons, in Angstroms.

* "-1" must be written at the end of atomic coordinates group.

4) Last line:

* The Z(atom-1') line must be as same as the first line, i.e. Z(atom-1) line, EXCEPT the value of zpos(1').

* The value of zpos(1') must be the distance between the (0,0,0) atom, which corresponds to the position of Z(atom-1), and the (u,v,w) atom.

Note: The sliced planes are perpendicular to the line which is formed by connecting the (0,0,0) atom to the (u,v,w) atom.

\$3. Example of input data file

The following example of the autoslice data simulates a convergent beam TEM image of silicon (Si) which has a diamond structure with a cubic unit cell of a=5.43 Angstroms.

The autoslice input data file, Si100.XYZ, for the layers of Si (Z=14), which are planes perpendicular to the line connecting the (0,0,0) atom to the (1,0,0) atom, is as follows;

The "wobble(i)" are 0.076 and sliced planes are perpendicular to <100>.

one unit cell of silicon <100>

5.43	5.43	5.43			
14	0.0000	0.0000	0.0000	1.0	0.076
14	2.7150	2.7150	0.0000	1.0	0.076
14	1.3575	4.0725	1.3575	1.0	0.076
14	4.0725	1.3575	1.3575	1.0	0.076
14	2.7150	0.0000	2.7150	1.0	0.076
14	0.0000	2.7150	2.7150	1.0	0.076
14	1.3575	1.3575	4.0725	1.0	0.076
14	4.0725	4.0725	4.0725	1.0	0.076
-1					
14	0.0000	0.0000	5.4300	1.0	0.076

CHAPTER III: Common

\$1. TIFF to Bitmap conversion

This application software has a function to convert the obtained tiff (TIF) file to a bitmap file and to review the bitmap (BMP) file.

Note: Only TIF file with version 6 format is supported for the conversion.

\$2. Others

On making sliced planes (which are perpendicular to the selected crystal direction <uvw>) and input data files for the atomic potential and the autoslice, it would be better to use “Multislice Assistance” software.

An example of sliced planes by “Multislice Assistance” is as follows;

(Note: Input data files for the atomic potential and autoslice are not shown here.)

Planes perpendicular to <1 1 1>

