

Quick userguide to mbfit in EDM

Mbfit is a simulation package for Many-beam Bloch wave calculation, which is originally written by K. Tsuda. The details of theory will not be presented here. The main features of mbfit include:

1. Convergent beam electron diffraction (CBED) simulation
2. Bloch state calculation
3. Dispersion surface calculation
4. Refinement of structure parameters using CBED experimental data

Currently only the first three are implemented in EDM2.0-beta package. Let's start with a simple tutorial.

Step by step tutorial:

1. Get a sample input file s3.txt

```
%mkdir test
```

```
%cd test
```

```
%cp /usr/local/edm/s3.txt ./
```

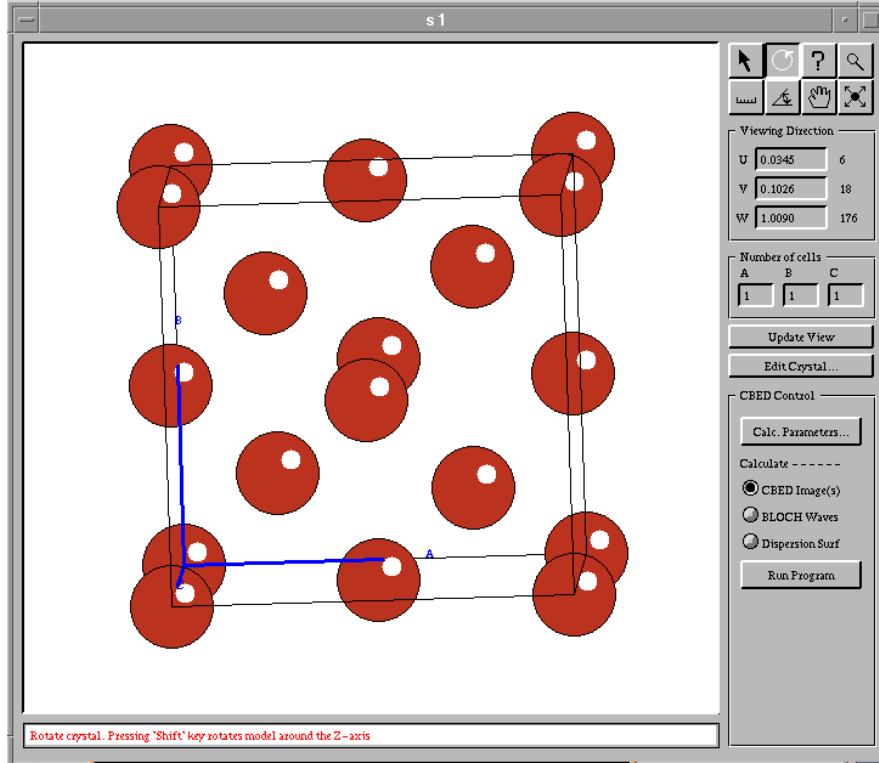
2. Launch edm

```
%edm
```

3. Select “open CBED file” under pull-down menu “File”

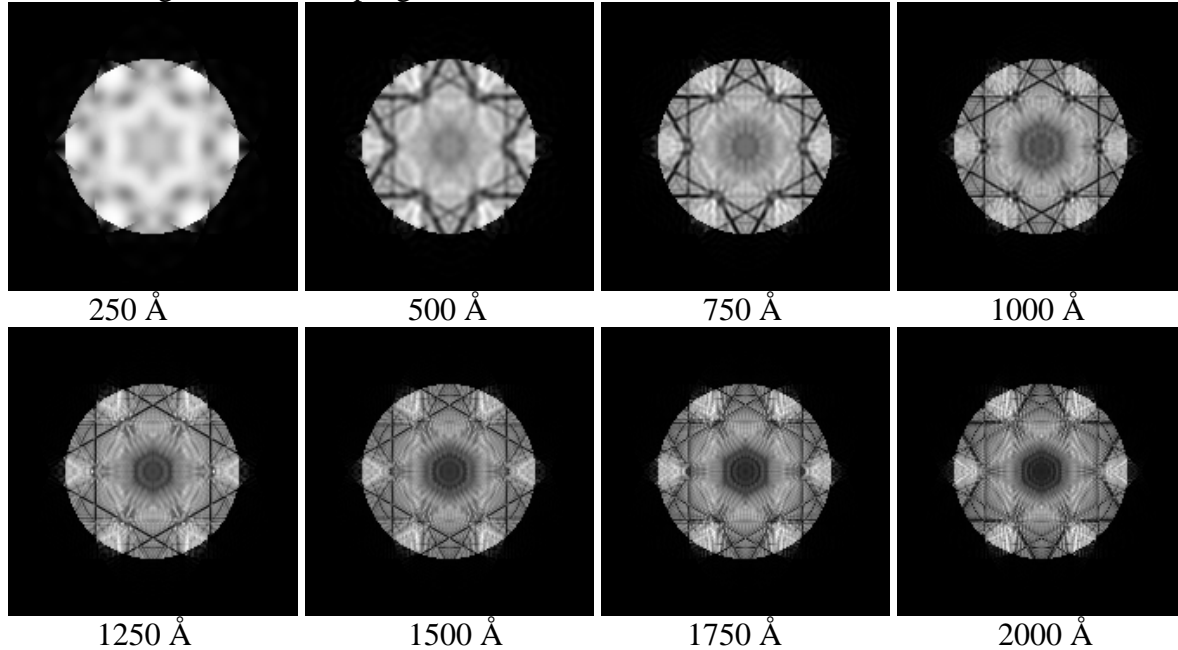
Choose the input file “s3.txt” and click “Ready”

You will see:



4. click “Run Program” button to run CBED simulation.

5. Image files in tif format are generated under /test directory. You can open those tif files using edm or other programs:



Anatomy of the input file for mbfit

The mbfit ignores comment characters followed by “#” or “%” in an input file. The input file is consists of four main datablocks and their sub-datablocks. Any data in the COMMENT{ }COMMENT data block will also be ignored.

There some example input files under directory /usr/local/edm/mbfit/:

s1.txt, s2.txt, s3.txt, s3.txt: CBED simulations

bl1.txt, bl2.txt: Bloch wave.

ds.txt: Dispersion surface

Theree IMPORTANT notes about input file format

1. The input file should be in *unix* format. If you edit the input file under DOS or windows, please convert them to unix text format by:

%dos2unix *.txt

2. **NO** space before keywords such as *LATTICE*{, }*LATTICE*, *ATOM*{, etc.

3. The *CALC_KXY_RANGE*{ }*CALC_KXY_RANGE* block should always before the *BEAM_SEARCH*{ }*BEAM_SEARCH* block.

The above input files are all annotated with self-explained text. All input files consist of 4 parts. Here are more details for them.

Part 1: Simulation mode

It tells mbfit to do what kind of simulation. The possible value is:

SIM_MODE #for CBED simulation

BLOCH_MODE #for Bloch wave calculation

DISPSURF_MODE *#for Dispersion surface calculation*

Part 2: Internal control parameter

Usually you don't need to change internal parameters. They are only useful for debugging the package. You can just leave it blank.

```
EPS_CONTROL_PARAMETERS{  
}EPS_CONTROL_PARAMETERS
```

Part 3: Crystal structure data block

This data block contains unit cell and atom sites information. It has three sub-datablocks: LATTICE, ATOM, and LOW_ORDER_FG. This data block is the same for CBED simulation, Bloch Wave calculation and Dispersion surface calculation.

An example for cubic SiC:

```
CRYSTAL_STRUCTURE_DATA{  
#  
LATTICE{  
216      # Number of space group  
# lattice parameter [in Angstrom units]  
4.358    # a  
4.358    # b  
4.358    # c  
90.0     # alpha  
90.0     # beta  
90.0     # gamma  
}LATTICE  
#  
ATOM{  
2 # Number of independent sites.  
# if you have n independent sites,  
#then you should have n SITE{ }SITE sub-datablock.  
#  
SITE{  
SI  
0.0      # x (fractional coordinate)  
0.0      # y  
0.0      # z  
ISO      # ISO: isotropic-B / ANISO: anisotropic-B  
0.5      # B [A2]  
1.0      # occupancy [0.0-1.0]  
0        # f(structure factor) table (0:Mott+BK, 1:BK+BK)  
}SITE  
SITE{  
C  
0.25     # x (fractional coordinate)  
0.25     # y  
0.25     # z  
ISO      # ISO: isotropic-B / ANISO: anisotropic-B  
0.5      # B [A2]  
1.0      # occupancy [0.0-1.0]  
0        # f(structure factor) table (0:Mott+BK, 1:BK+BK)  
}SITE  
  
}ATOM  
#  
LOW_ORDER_FG{
```

```

# this is for refinement of structure parameters mode.
# just leave it as 0
# Nothing to do CBED simulation, Bloch wave, and Dispersion surface modes
0    # number of low-order g, this is for refinement of structure parameter
}LOW_ORDER_FG
}CRYSTAL_STRUCTURE_DATA

```

Part 4: Simulation conditions data

This data block contains information for simulation conditions, such as incidence beam, accelerating voltage, thickness etc. Note that for different simulation modes, this data block has different sub-datablocks.

4.1 An example for CBED

```

SIM_CALCULATION_CONDITION{
#
INCIDENT_BEAM{
1  1  1    # Incidence      (upward)
1  1  1    # Surface normal (upward)
2 -2  0    # ZOLZ base vector
0.0        # H tilt
0.0        # G tilt
100.0      # Accelerating Voltage [kV]
}INCIDENT_BEAM
#
CALC_KXY_RANGE{
0    # cal_range_flag [dummy: always 0]
2    # Calc. type [0:0D, 1:1D, 2:2D disk, 3:2D square]
# Calc. type: 0 for Bloch waves, 1 for Dispersion surface
# Calc. Type: 2 and 3 for CBED simulation.
101  # numh: number of calc. points > 5 (total~sq(numh))
#the final image will be 101x101
-3.0 3.0    # h_begin, h_end
-3.0 3.0    # g_begin, g_end
}CALC_KXY_RANGE
#
BEAM_SEARCH{
# Automatic beam search
2          # Beam search method [0>manual, 1:auto[wg], 2:[sg]]
400 4.0 0 0    # num_g_limit, g_max[A^{-1}], LaueZone_min, LaueZone_max
# num_g_limit: maximum number of g
# if you want to search higher Lauezones, set LaueZone_max>0
0.02 0.03 1e+11 # S_g_exact_max, S_g_bethe_max,  $\xi_g$ _max
# if the beam search method is 1, then the above line is W_g_exact_max, W_g_bethe_max,  $\xi_g$ _max
}BEAM_SEARCH
#
OUTPUT_REFLEX{
2 # Number of reflections to be calculated (0:all)
# indices hkl
0 0 0
2 -2 0
#
}OUTPUT_REFLEX
OUTPUT_THICKNESS{
# Number of thicknesses for output
2

```

```
# thicknesses (in Angstrom units)
250
500
}OUTPUT_THICKNESS
}SIM_CALCULATION_CONDITION
```

4.2 An example for Bloch wave

```
BLOCH_CALCULATION_CONDITION{
#
INCIDENT_BEAM{
1 1 1 # Incidence (upward)
1 1 1 # Surface normal (upward)
2 -2 0 # ZOLZ base vector
-1.0 # H tilt
0.0 # G tilt
100.0 # Accelerating Voltage [kV]
}INCIDENT_BEAM
#
CALC_KXY_RANGE{
0 # cal_range_flag [0:manual]
0 # Calc. type [0:0D], 0 for Bloch wave
1 # numh: number of calc. points
0.0 0.0 # h_begin, h_end
0.0 0.0 # g_begin, g_end
}CALC_KXY_RANGE
#
BEAM_SEARCH{
# Automatic beam search
2 # Beam search [0:manual, 1:automatic-wg, 2:automatic-sg]
200 4.0 0 0 # num_g_limit, g_max[A^{-1}], LaueZone_min, LaueZone_max
# if you want to search higher Lauezones, set LaueZone_max>0
0.02 0.03 1e+11 # S_g_exact_max, S_g_bethe_max,  $\zeta_g$ _max
}BEAM_SEARCH
#
CALC_RXY_RANGE{
101 101 # Number of calculation points for x, y (odd number)
-2.0 2.0 # x_begin, x_end (along the ZOLZ base vector)
-2.0 2.0 # y_begin, x_end (perpendicular to the ZOLZ base vector)
}CALC_RXY_RANGE
#
OUTPUT_BRANCH{
1 7 # Number of branches to be calculated (begin, end)
}OUTPUT_BRANCH
}BLOCH_CALCULATION_CONDITION
```

4.3 An example for Dispersion surface

```
DISPSURF_CALCULATION_CONDITION{
#
INCIDENT_BEAM{
1 1 1 # Incidence (upward)
1 1 1 # Surface normal (upward)
2 -2 0 # ZOLZ base vector
0.0 # H tilt
0.0 # G tilt
100.0 # Accelerating Voltage [kV]
}INCIDENT_BEAM
```

```

#
CALC_KXY_RANGE{
0      # cal_range_flag [dummy: always 0]
1      # Calc. type [should be 1 for DISPSURF_MODE]
81     # numh: number of calc. points > 5 (total~sq(numh))
-2.0  2.0      # h_begin, h_end
0.0   1.0      # g_begin, g_end
}CALC_KXY_RANGE
#
BEAM_SEARCH{
# Automatic beam search
2          # Beam search [0>manual, 1:automatic-wg, 2:automatic-sg]
200  4.0  0  0      # num_g_limit, g_max[A^{-1}], LaueZone_min, LaueZone_max
# if you want to search higher Lauezones, set LaueZone_max>0
0.02  0.03  1e+11 # S_g_exact_max, S_g_bethe_max,  $\xi_g$ _max
}BEAM_SEARCH
#
OUTPUT_BRANCH{
1  7      # Number of branches to be calculated (begin, end)
}OUTPUT_BRANCH
#
OUTPUT_REFLEX{
2          # Number of reflections (0 means no output of epsCg and intensities)
# indices hkl
0 0 0
2 -2 0
}OUTPUT_REFLEX
#
OUTPUT_THICKNESS{
2      # Number of thicknesses for output # (0: no intensity output)
# thicknesses (Angstrom)
250
500
}OUTPUT_THICKNESS
}DISPSURF_CALCULATION_CONDITION

```

Attached is an input file s1.txt which is for CBED simulation:

```
#
# mbfit: a sample data for CBED simulation
# Comment lines:  # or % or COMMENT{  }COMMENT
#
# -----
# the data block 1: simulation mode
# job type
# SIM_MODE: CBED simulations
# BLOCH_MODE: Bloch waves
# DISPSURF_MODE: Dispersion surface
#
SIM_MODE
#
# end of part 1
# -----
#
#-----
# part 2: internal control parameters
# just leave it blank, you don't need to change them
#
EPS_CONTROL_PARAMETERS{
}EPS_CONTROL_PARAMETERS
#
# end of part 2
# -----
#
#-----
# part 3: crystal structural data block
#
CRYSTAL_STRUCTURE_DATA{
#
LATTICE{
227      # Number of space group
# lattice parameter [in Angstrom units]
5.43     # a
5.43     # b
5.43     # c
90.0     # alpha
90.0     # beta
90.0     # gamma
}LATTICE
#
ATOM{
1  # Number of independent sites.
# if you have two independent sites,
#then you should have two SITE{ }SITE sub-datablock.
#
SITE{
SI
0.0      # x (fractional coordinate)
0.0      # y
0.0      # z
ISO      # ISO: isotropic-B / ANISO: anisotropic-B
```

```

0.5      # B [A{2}]
1.0      # occupancy [0.0-1.0]
0        # f(structure factor) table (0:Mott+BK, 1:BK+BK)
}SITE
}ATOM
#
LOW_ORDER_FG{
0        # number of low-order g
}LOW_ORDER_FG
}CRYSTAL_STRUCTURE_DATA
#
# end of part 3
# -----

#
# -----
# part 4: Simulation conditions
#
SIM_CALCULATION_CONDITION{
#
INCIDENT_BEAM{
1  1  1      # Incidence      (upward)
1  1  1      # Surface normal (upward)
2  -2  0      # ZOLZ base vector
0.0          # H tilt
0.0          # G tilt
100.0        # Accelerating Voltage [kV]
}INCIDENT_BEAM
#
CALC_KXY_RANGE{
0        # cal_range_flag [dummy: always 0]
2        # Calc. type [0:0D, 1:1D, 2:2D disk, 3:2D square]
101      # numh: number of calc. points > 5 (total~sq(numh))
-1.0  1.0    # hbgn, hend
-1.0  1.0    # gbgn, gend
}CALC_KXY_RANGE
#
#
BEAM_SEARCH{
# Automatic beam search
2          # Beam search [0>manual, 1:automatic-wg, 2:automatic-sg]
200  4.0  0  0      # num_g_limit, g_max[A{-1}], lz_min, lz_max
0.02  0.03  1e+11  # sg_exact_max, sg_bethe_max, xi_g_max
}BEAM_SEARCH
#
COMMENT{ -----
BEAM_SEARCH{
# Manual beam input
0        # Beam search method [0>manual, 1:auto[wg], 2:[sg]]
7  0      # num. of exact, num. of bethe
0        0        0      # hkl
2        -2       0
-2       2        0
2        0        -2
-2       0        2
0        2        -2
0        -2       2

```



```
}BEAM_SEARCH
}COMMENT -----
#
OUTPUT_REFLEX{
2  # Number of reflections to be calculated (0:all)
# indices hkl
0 0 0
2 -2 0
#
}OUTPUT_REFLEX
OUTPUT_THICKNESS{
# Number of thicknesses for output
2
# thicknesses (in Angstrom units)
250
500
}OUTPUT_THICKNESS
}SIM_CALCULATION_CONDITION
# end of part 4
#-----
```