How to use Wsr : Electromagnetic field simulator by RCWA

1. Preparation before use and use conditions

1．Operating environment (supported OS): Windows 64bit 7,8,10,11 Edition

2．Status at the time of distribution

Included files

- Ws_soft
  - Wsems → Wsems.exe, HScrollListbox.dll, Wsbch.exe, Wscnt.exe, Sup.exe(1) Wsf.exe, Wsr.exe, Wsb.exe, Afm.exe, Ems.exe nk.dat, sub.dat
    - Picture → 1_a1.png etc.
    - Text → wsb_j.txt, wsf_j.txt, wsr_j.txt , wsb_e.txt, wsf_e.txt, wsr_e.txt
  - Install → w_ifort_runtime_p_2022.2.0.3790.exe
  - Samples
    - 220401-cnt&mnt → i_xz.out, i_xz_t.out, i_xy.out, m_xz.out, m_xy.out, i_far.out
    - 220401-wsb → wsb01.dat～wsb13.dat
    - 220401-wsf → wsf01.dat～wsf14.dat
    - 220401-wsr → wsr01.dat～wsr17.dat
    - Comparison
      - 230208-wsb → wsb_1.dat～wsb_9.dat
      - 230208-wsf → wsf_1.dat～wsf_9.dat
      - 230208-wsr → wsr_1.dat～wsr_9.dat
    - → nk_data.xlsx, sub_data.xlsx, nk.dat, sub.dat
  - → Wsems.exe_shortcut, ReadMe.txt

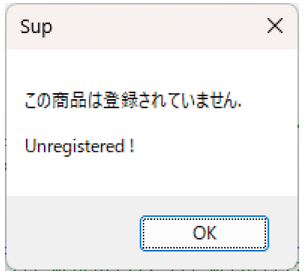
(note 1) Sup.exe is a file for determining registration, which should be stored in the same folder Wsems as other exe files.

3．Installation Procedure

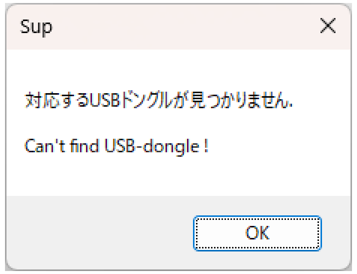
3.1 Copy the folder Ws_soft to a drive (e.g., drive D).

3.2 Click on w_ifort_runtime_p_2022.2.0.3790.exe to install the runtime.

①



②



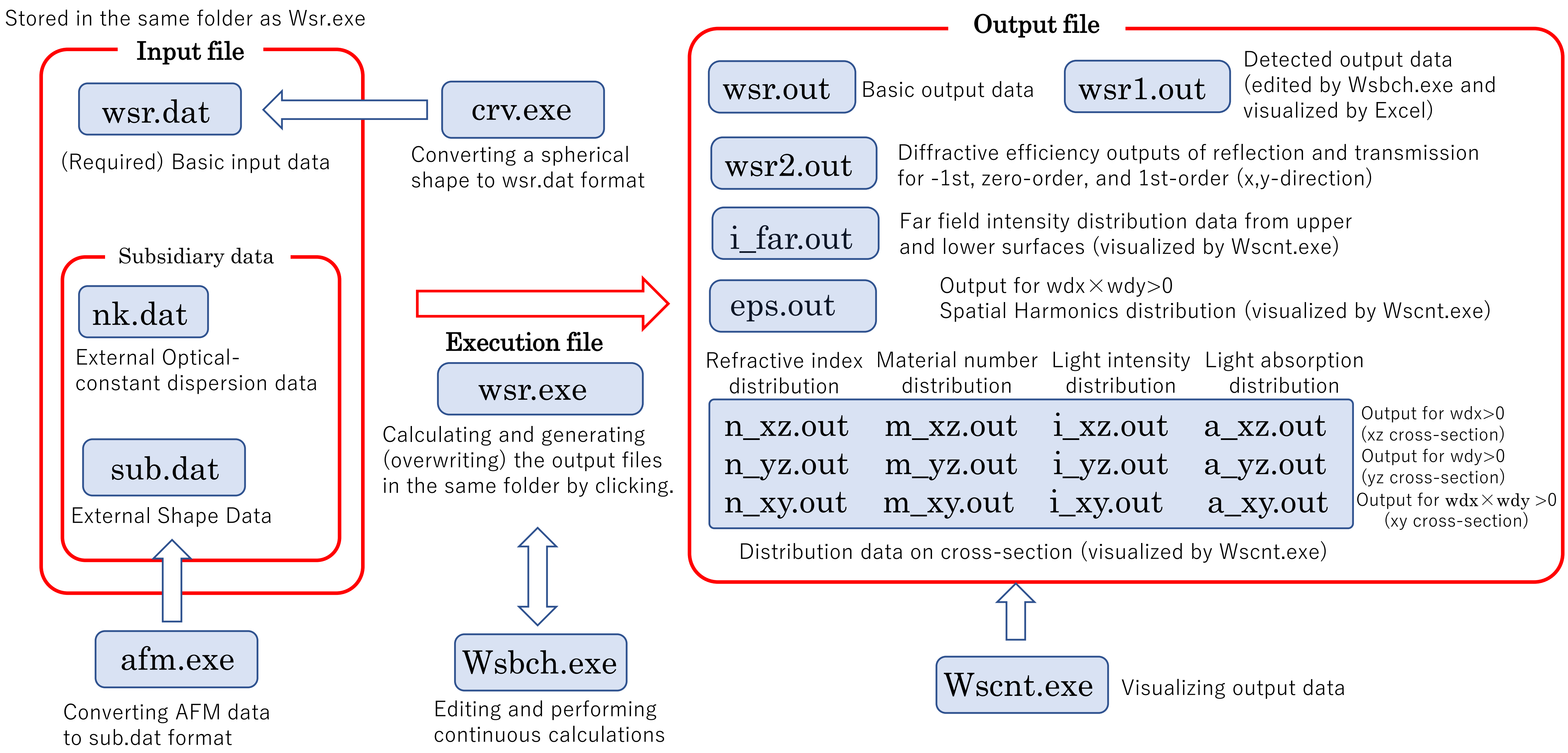
4．Uninstallation procedure

Delete the folder Ws_soft.

5．Restriction on use

- If a registered USB dongle is connected (or MAC address is registered) and the corresponding sup.exe is installed in the folder “Wsems”, calculation starts without any function restrictions.
- If the sup.exe included in the folder “Wsems” does not correspond to the registered USD dongle or registered MAC address, the message ① is displayed for 5 seconds. If the USB dongle is not connected, the message ② is displayed for 5 seconds. Air and two optical materials limit applies. However, to the extent that use is within the limit, the calculation continues.

2. Input/output and relationships between other software



3. Contents of output files

wsr.out : Main calculation results. Transmitted (light amount flowing out from +z boundary surface of the analysis area), Reflected (light amount flowing out from -z boundary surface), Absorbed_M01(light amount flowing in from all boundaries of specified material 01, i.e., absorbed light amount),M01_ - x to +z (light amount flowing in from each boundary of specified material 01).

wsr1.out : Extracted calculation results : Transmitted (light amount flowing out from +z boundary surface of the analysis area), Reflected (light amount flowing out from -z boundary surface), Absorbed_M01(light amount flowing in from all boundaries of specified material 01, i.e., absorbed light amount),Inflow_M01_ - x to +z (light amount flowing in from each boundary of specified material 01).

wsr2.out : Extracted calculation results, diffraction efficiencies for diffraction orders from -1st to +1st. R(? , ?) : Reflective diffraction efficiency (order in x-direction, order in y-direction), T(? , ?) : Transmissive diffraction efficiency (order in x-direction, order in y-direction).
m_xy.out : xy cross-sectional distribution of material numbers. The results of the upper and lower boundary surfaces of each layer are overlayed from the -z side to the +z side. **m_xz.out** : xz cross-sectional (y = csy) distribution of material numbers. **m_yz.out** : yz cross-sectional (x = csx) distribution of material numbers. **m_z045.out** : cross-sectional distribution with 45-degrees rotation around z-axis for material numbers. **m_z135.out** : cross-sectional distribution with 135-degrees rotation around z-axis for material numbers. These images can be displayed by Wscnt.

n_xy.out : xy cross-sectional distribution of refractive indexes. The results of the upper and lower boundary surfaces of each layer are overlayed from the -z side to the +z side. **n_xz.out** : xz cross-sectional (y = csy) distribution of refractive indexes. **n_yz.out** : yz cross-sectional (x = csx) distribution of refractive indexes. **n _z045.out** : cross-sectional distribution with 45-degrees rotation around z-axis for refractive indexes. **n_z135.out** : cross-sectional distribution with 135-degrees rotation around z-axis for refractive indexes. These images can be displayed by Wscnt.

k_xy.out : xy cross-sectional distribution of extinction coefficients. The results of the upper and lower boundary surfaces of each layer are overlayed from the -z side to the +z side. **k_xz.out** : xz cross-sectional (y = csy) distribution of extinction coefficients. **k_yz.out** : yz cross-sectional (x = csx) distribution of extinction coefficients. **k_z045.out** : cross-sectional distribution with 45-degrees rotation around z-axis for extinction coefficients. **k_z135.out** : cross-sectional distribution with 135-degrees rotation around z-axis for extinction coefficients. These images can be displayed by Wscnt.

i_xy.out : xy cross-sectional distributions of light intensity (i. e., magnitude of Poynting vector※). The results for the upper and lower surfaces of each layer are superimposed from the -z side to the +z side. **i_xz.out** : xz cross-sectional (y=csy) distributions of light intensity. **i_yz.out** : yz cross-sectional (x=csx) distributions of light intensity. **i_z045.out** : cross-sectional distribution with 45-degrees rotation around z-axis for light intensity. **i_z135.out** : cross-sectional distribution with 135-degrees rotation around z-axis for light intensity. These images can be displayed by Wscnt.

a_xy.out : xy cross-sectional distributions of absorption. The results for the upper and lower surfaces of each layer are superimposed from the -z side to the +z side. **a_xz.out** : xz cross-sectional (y=csy) distributions of absorption. **a_yz.out** : yz cross-sectional (x=csx) distributions of absorption. **a_z045.out** : cross-sectional distribution with 45-degrees rotation around z-axis for absorption. **a_z135.out** : cross-sectional distribution with 135-degrees rotation around z-axis for absorption. These images can be displayed by Wscnt.

i_far.out : Far-field intensity distributions (-z side and +z side in the order). The image can be displayed by Wscnt.

eps.out : Spatial harmonics distribution. Calculated results for all layers are superimposed. The image can be displayed by Wscnt.

※ For ity=0, Intensity is a magnitude of Poynting vector, for ity=1, an electric and magnetic filed intensity, for ity=2, an electric filed intensity, and for ity=3, a magneticfiled intensity.

4. Execution method

Among the three methods, we strongly recommend (1) because it allows setting numerical data without worrying about input rules.

(1) Method by using wsems.exe (most recommended). In detaile, see “How to use Wsems”.

(2) Method by clicking wsb.exe directly

Wsems —— Wsr.exe, wsr.dat
Samples —— 220401-wsr —— wsr01.dat

Rename, overwrite, and click Wsr.exe

The vertical alignment of wsb.dat is easier to be edited if the font is set to Courier New in Notepad. However, note that it is not possible to distinguish between full-width and half-width spaces.

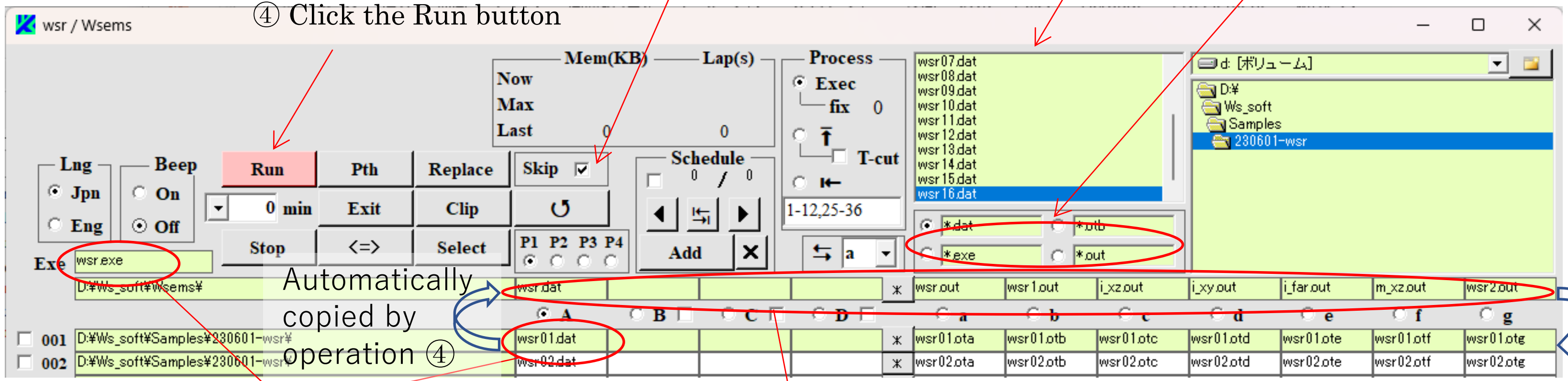
(3) Method using wsbch.exe (steps ① to ④ below)

③ Uncheck the box

File list box

File pattern

④ Click the Run button



Automatically copied by operation ④

Automatically copied after calculations are completed

① After clicking the box and selecting the file pattern, select the wsr.exe and wsr01.dat files from the file list.

② At first, write directly such like “wsr.dat” after clicking the boxes of A or a - g. After the second time, they are automatically listed.

5. Method of drawing calculation results

During the calculation, wscnt in the same folder start in linkage with the execution of wsr.exe, and the calculation results of i_xz.out or i_yz.out are displayed in real time.

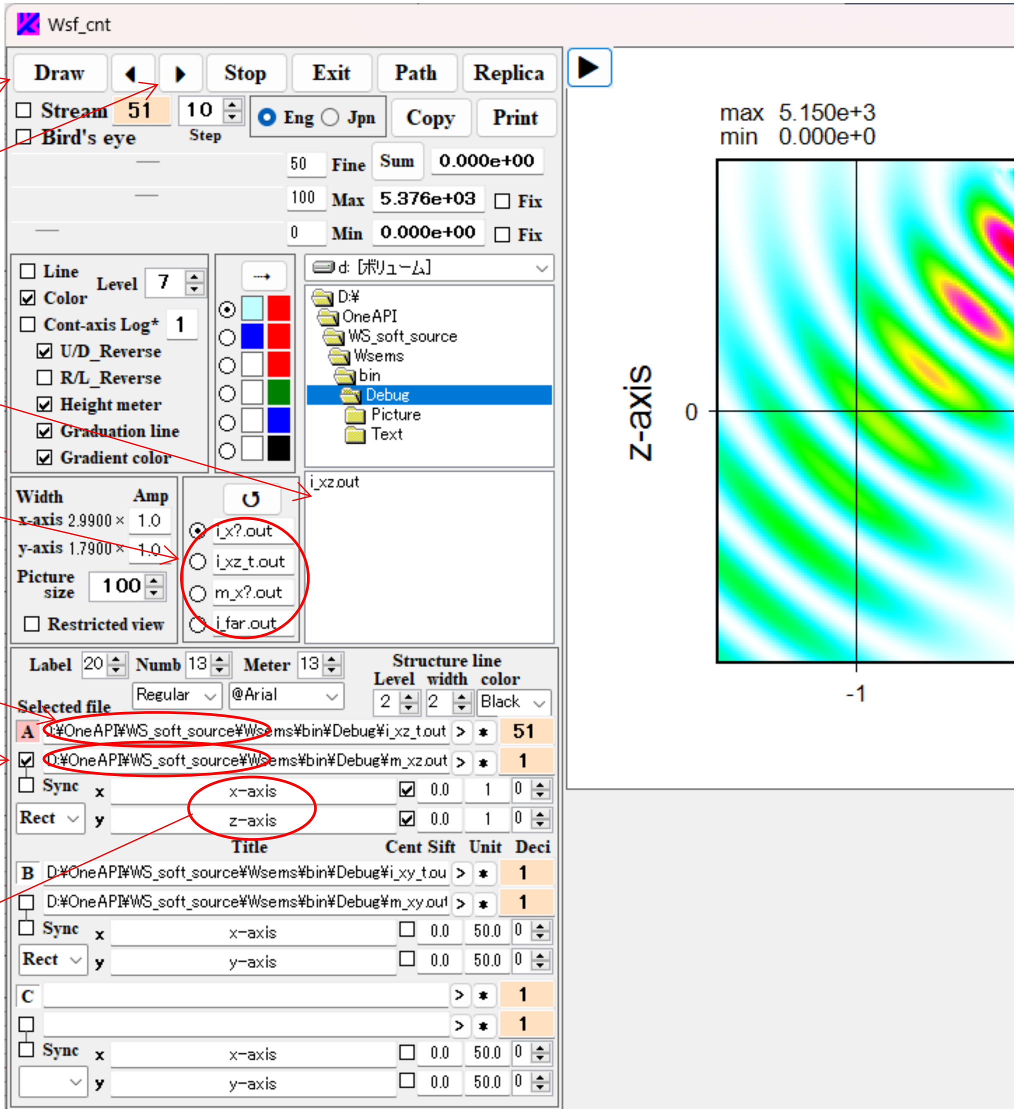
④Click Draw button to start drawing.
⑤Click ▶ button to advance frame.

File list box

File pattern

①After click the box, select a file pattern, and choose the file from the file list box.
② To add a structure line, check the checkbox and click the box on the right and select the file from the file list box.
③ Click on the box and type in directly.

Output data generated in ¥Ws_soft¥Wsems can be visualized by wscnt.exe in the steps ①~⑤. If registered, limitation of file patterns is removed and "ot?" files generated by wsbch can also be visualized.



6. Input rules for input file (wsr09.dat)

The following pages can be ignored when using Wsems.

Numeric data input rules

- Input numbers must be one-byte numbers. A space is a half-width space, and Tab code is not acceptable.
- The right end of the input numerals should be aligned with the vertical line on the right end of the variable label (or the * mark) above.
- The number without a decimal point is an integer type, and that with a decimal point (5 or less digits) is a real number type.

```
Digit 1        10        20        30        40        50
  ** wsr.dat
① *        hm       trc    wb(um)  kfl(0,1)  kot       ity
          5.0       1.0       0.0         0    0         0
② *   wdx(um)   wdy(um)   dxy(um)    dz(um)
          3.0       0.0      0.01      0.01
  *   Lam(um)   th(deg)   fi(deg)   gm(deg)
         0.94       0.0       0.0       0.0
  *       alx       aly   sx0(um)   sy0(um)
          0.3       0.3       0.0       0.0
  *   stx(um)   sty(um)   csx(um)   csy(um)
          0.5       0.0       0.0       0.0
③ * km   *   Name   ko        an        ab        ak
     1      Ta205    1    1.0000      0.00    0.0000
     2        -Al    1    1.4500      0.00    0.0000  Digit60        70        80        90       100       110
  * kr      * kd   kt   ps(deg)    px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)        xp
     1#        0    4       0.0      1.50      1.50     0.500      0.50      0.00      0.00       0.0
  * kf   km   kr kd   kt   ps(deg)    px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)        xp        xq
     1    1    0  0    2       0.0      0.00      0.00      0.50      0.50     0.000      0.00       0.0       0.0
     2    2    0  0   -2       0.0      0.00      0.00      0.60      0.60     0.000      0.00       1.0       0.0
④ * kb   kl   km   kp        tk   kf    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
     1    0    0    0      0.40    0    0
     2    0    0    0      0.50    1    0
     3    0    0    0      0.10    1    2
     4    0    0    0      0.50    1    0
```

Examples of incorrect input.

①
```
*        hm       trc    wb(um)
       ５.00      1.00   　0.500
```
Full-width digit. A full-width space is contained.

②
```
*   wdx(um)   wdy(um)   dxy(um)
      1.500    1.500      0.020
```
The right edge of the input number deviates from the right of the variable label above.

③
```
* km   *     Name   ko        an
   1   Ta205        1.0        1
```
Beyond the 8-column range. Real number type is put into integer type. Integer type is put into real number type.

④
```
* kb  kl  km  kp      tk  kf   *
   1   0   0   0    0.40   0   0
   2   0   0   0    0.50   1   0
   3   0   0   0    0.10   1    2
   4   0   0   0    0.50   1   0
```
The right edge of the input number deviates from position of the * mark above.

```
* kb  kl  km  kp      tk  kf   *
   1   0   0   0    0.40   0   0
   2   0   0   0    0.50   1   0
   3   0   0   0    0.10   1   2
c
   4   0   0   0    0.50   1   0
```

To interrupt a calculation in the middle of layers, insert a line leading "C" at the interruption position.

7. Contents of wsr.dat (wsr01.dat), Compute time 2.2s

Calculations are in a convergence process for 4~7, and in a near convergence for more than 20. When a metal is included, calculation convergence oscillates.

In the case of metals, the convergence is slightly less oscillatory than for even.

```
Digit 1      10         20         30         40         50      Digit60        70          80          90         100         110
 ** wsr.dat
 *        hm        trc         wb(um)    kfl(0,1)   kot                      ity
          5.0        2.0         0.0          0          0                      0
 *       wdx(um)    wdy(um)    dxy(um)     dz(um)
          1.5        1.5        0.01       0.01
 *       Lam(um)     th(deg)    fi(deg)    gm(deg)
         0.75        0.0        0.0        0.0
 *       alx        aly         sx0(um)    sy0(um)
          1.0        1.0        0.0        0.0
 *       stx(um)    sty(um)    csx(um)    csy(um)
          0.0        0.0        0.0        0.0
 * km    *    Name  ko          an         ab          ak
     1#      Ta205   1      1.0000       0.00      0.0000
     2        -Al    1      1.4500       0.00      0.0000
 * kr          * kd    kt       ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)     xp
     1#           0     4       0.0        1.50       1.50      0.500       0.50       0.00       0.00      0.0
 * kf    km   kr kd    kt       ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)     xp          xq
     1    2    0  0     1       0.0        0.00       0.00       0.50       0.50      0.000       0.00      0.0         0.0
     2#   2    0  0    -2       0.0        0.00       0.00       0.60       0.60      0.000       0.00      1.0         0.0
 * kb   kl   km   kp        tk     kf     *     *     *     *     *     *     *     *     *     *     *     *     *
     1    0    0    0      0.25     0     0
     2    0    0    0      0.10     1     0
     3    0    0    0      0.25     0     0
```

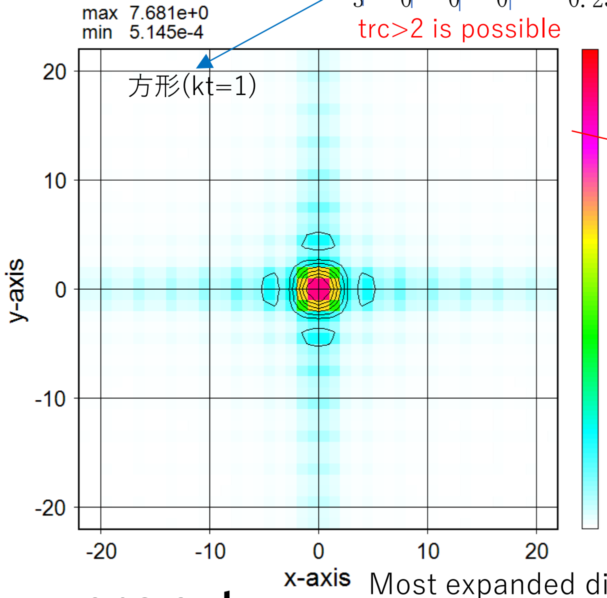
Sequential numbers must be assigned from 1 (no more than 4 digits)

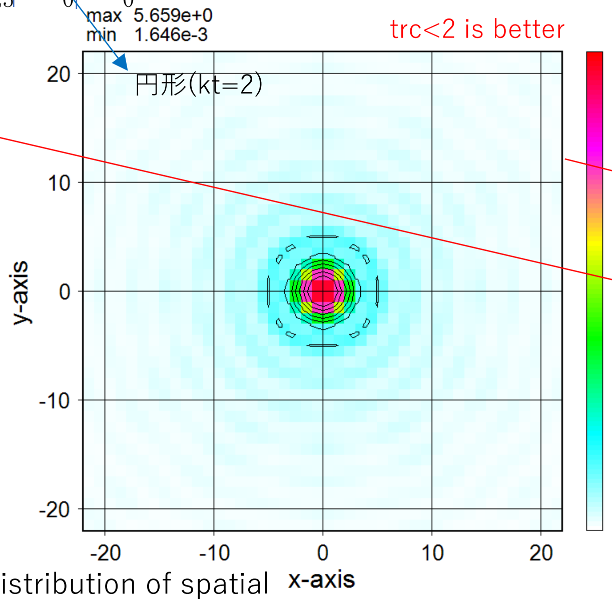
hm	Harmonic Number Ratio. The larger the absolute value, the more accurate, but the greater the computational load. Normally set to 4.0 to 7.0. >0 : Harmonics number is an odd value, rounding up |hm|*(wdx+2*wb)/Lam or |hm|*(wdy+2*wb)/Lam. <0: Harmonics number is an even value (i.e., cited odd value -1).
trc	Truncation factor (>=0) that works only for 3-D problems. If =0, it is treated as no truncation. The smaller the coefficient, the more accurate, but the greater the computational load. Normally set to 1.0 to 3.0.

The optical shape represented by the refractive index distribution reflects the spatial harmonics distribution (eps.out) of the electromagnetic coefficient ε on the xy-section, with square shapes having a cross-shaped distribution and circular shapes having a concentric circle distribution (see "Calculation Principles and Examples"). The cross-shaped distribution corresponds to trc=10 and the concentric circle distribution corresponds to trc=1.0, and the size of trc can be predicted by the distribution shape.

Large error Small memory consumption Small calculation time	⟷	Small error Large memory consumption Large calculation time

hm	h	5	7	10
Matrix size (1D)	h	0.71	1	1.43
Matrix size (2D) = Memory size or Computing time	h^2	0.51	1	2.04
trc	**>10**	**2.0**	**1.0**	**0.0**
Shape of spatial harmonics (eps.out)				
Matrix size (1D)	<0.1	0.5	$\pi/4$	1
Matrix size (2D)	$<0.1^2$	0.5^2	$(\pi/4)^2$	1



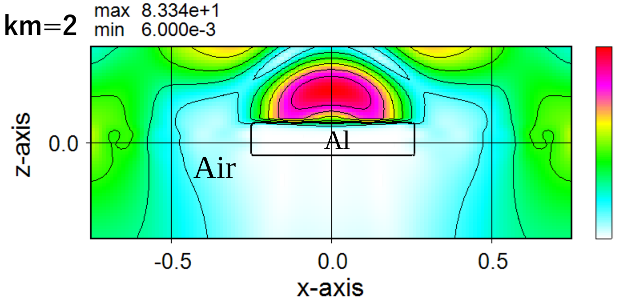


eps.out

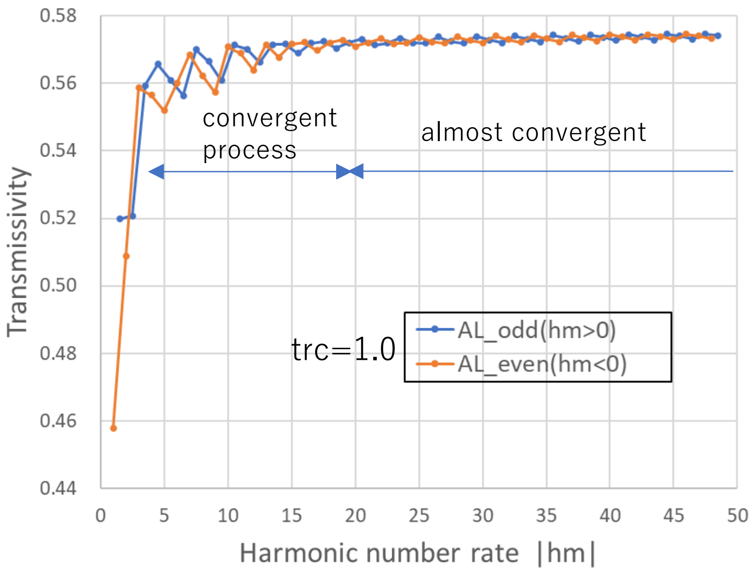
Most expanded distribution of spatial harmonics, visualized in 2nd Wscnt.

8. Contents of wsr.dat (wsr02.dat), 0.7s

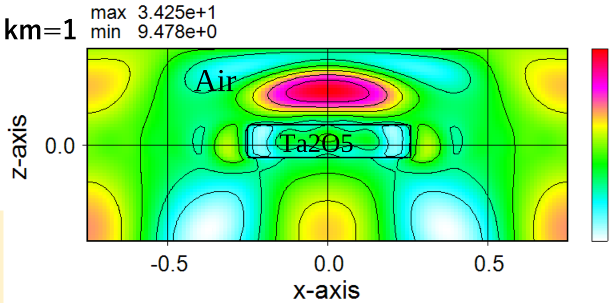
```
Digit 1        10        20        30        40        50
** wsr.dat
*         hm       trc        wb(um)    kf1(0,1)   kot        ity
         5.0       1.0        0.0        0          0          0
*       wdx(um)  wdy(um)    dxy(um)    dz(um)
         1.5       0.0       0.01       0.01
*       Lam(um)   th(deg)    fi(deg)    gm(deg)
        0.75       0.0        0.0        0.0
*         alx       aly      sx0(um)    sy0(um)
         1.0       1.0        0.0        0.0
*       stx(um)  sty(um)    csx(um)    csy(um)
         0.0       0.0        0.0        0.0
* km    *   Name  ko       an        ab        ak
   1#      Ta2O5   1    1.0000      0.00    0.0000
                                                     Digit60    70     80     90     100    110
   2         -Al   1    1.4500      0.00    0.0000
* kr       * kd   kt   ps(deg)   px(um)   py(um)   wx(um)   wy(um)   sx(um)   sy(um)   xp
   1#         0    4    0.0       1.50     1.50     0.500    0.50     0.00     0.00     0.0
* kf    km   kr kd   kt   ps(deg)   px(um)   py(um)   wx(um)   wy(um)   sx(um)   sy(um)   xp    xq
   1     2    0  0    2    0.0       0.00     0.00     0.50     0.50     0.000    0.00     0.0   0.0
   2#    2    0  0   -2    0.0       0.00     0.00     0.60     0.60     0.000    0.00     1.0   0.0
* kb  kl  km  kp     tk   kf   *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
   1   0   0   0   0.25    0   0
   2   0   0   0   0.10    1   0
   3   0   0   0   0.25    0   0
```



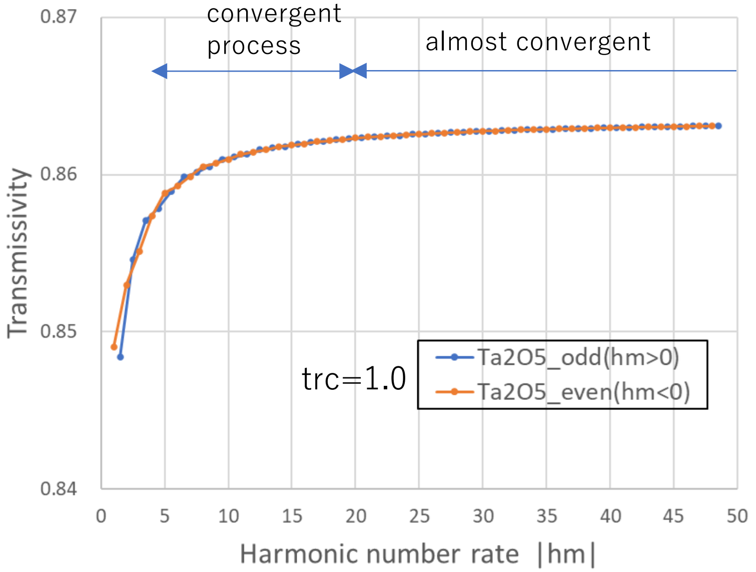
i_xz.out & m_xz.out



If hm and trc are set each large and small, the analysis results will approach the true value, but the computational load will increase significantly, so a compromise should be made where the change in the results for different values of hm or trc is small.



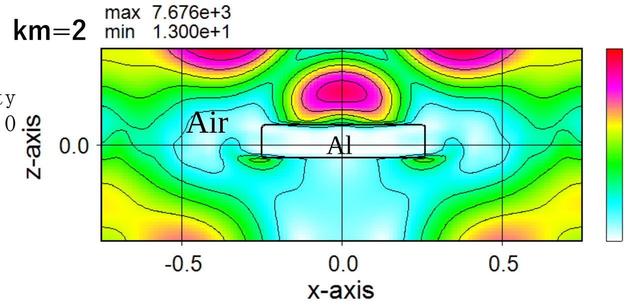
i_xz.out & m_xz.out



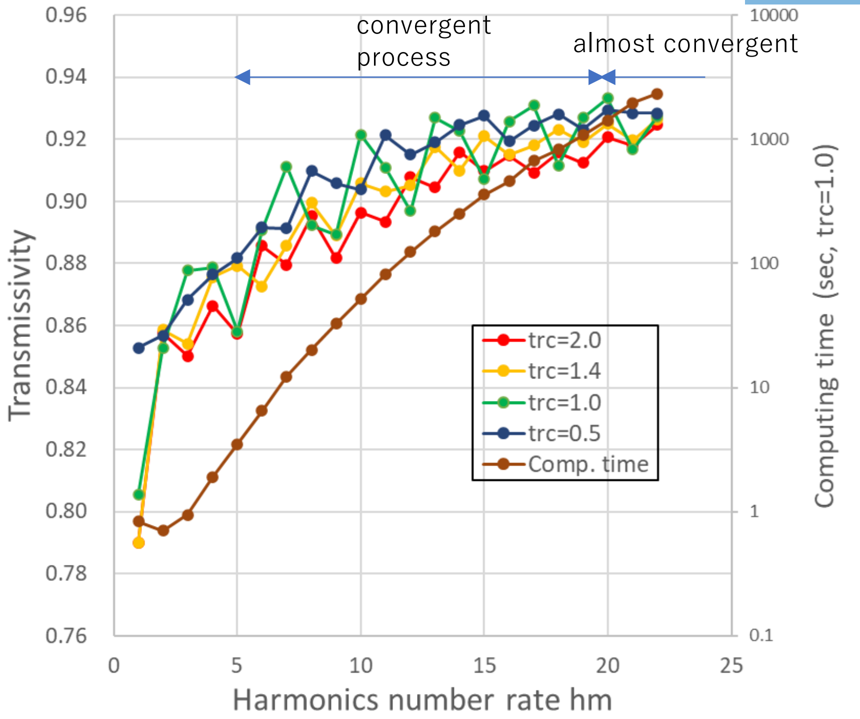
The RCWA method stands for rigorous coupled wave analysis, which has the modifier “rigorous,” but approximations exist, in reality, because the lower-order components of spatial harmonics are extracted to create a convolution matrix in the expression for a refractive index distribution. The extraction method is based on the limitation of diffraction orders (limitation of the harmonics number by hm), and in 3D analysis, the limitation in spatial orientation (limitation by trc) is also added. A size of trc can be estimated by the distribution shape of spatial harmonics (results of eps.out). In an actual use, hm = 4 to 7, trc=1.0 to 3.0.

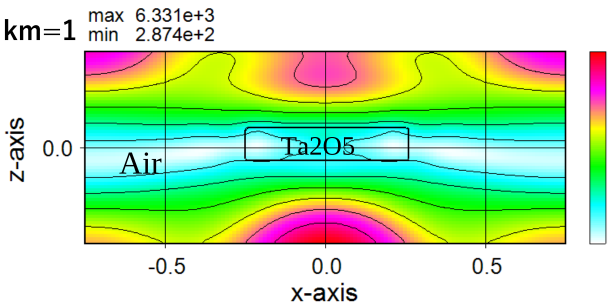
9. Contents of wsr.dat (wsr03.dat), 3s


```
Digit 1        10        20        30        40        50
** wsr.dat
*        hm       trc     wb(um)  kfl(0,1)      kot         ity
       5.00      2.00      0.000         0        0           0
*   wdx(um)   wdy(um)    dxy(um)    dz(um)
      1.500     1.500      0.010     0.010
*   Lam(um)   th(deg)    fi(deg)   gm(deg)
      0.750      0.00       0.00      0.00
*       alx       aly    sx0(um)   sy0(um)
       1.00      1.00      0.000     0.000
*   stx(um)   sty(um)    csx(um)   csy(um)
      0.000     0.000      0.000     0.000
*km    *     Name   ko        an        ab         ak
  1#         Ta2O5   1    1.0000      0.00     0.0000
  2            -Al   1    1.4500      0.00     0.0000  Digit60      70       80       90      100      110
*kr    *       kd   kt   ps(deg)    px(um)    py(um)   wx(um)   wy(um)   sx(um)   sy(um)      xp
  1#            0    4       0.0      1.50      1.50    0.500     0.50     0.00     0.00     0.0
*kf   km   kr   kd   kt   ps(deg)    px(um)    py(um)   wx(um)   wy(um)   sx(um)   sy(um)      xp      xq
  1    2    0    0    2       0.0      0.00      0.00     0.50     0.50    0.000     0.00     0.0     0.0
  2#   2    0    0   -2       0.0      0.00      0.00     0.60     0.60    0.000     0.00     1.0     0.0
*kbkl  km   kp     tk(um)   kf    *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *
  1     0    0       0.25    0    0
  2     0    0       0.10    1    0
  3     0    0       0.25    0    0
```

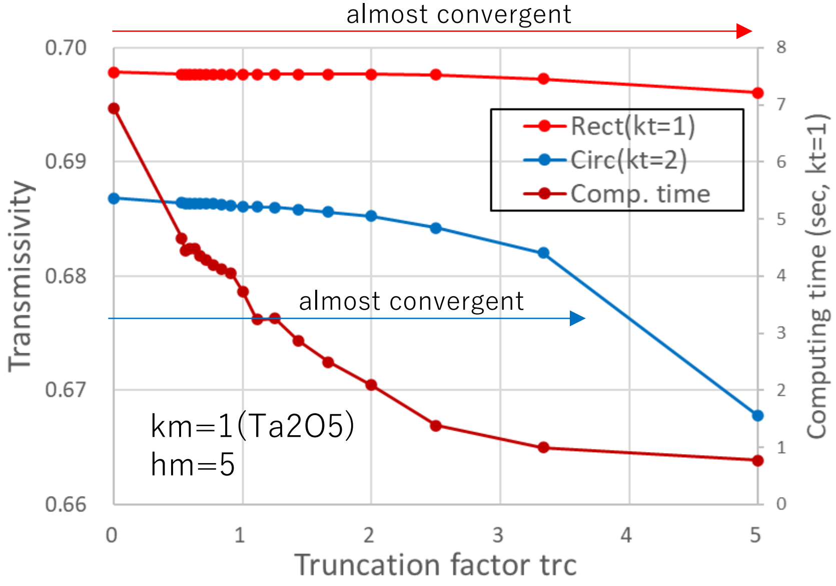


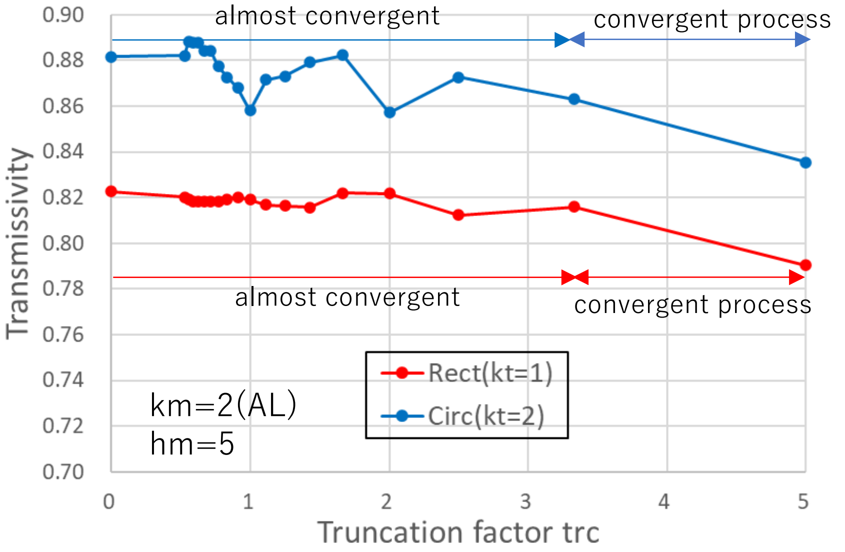
i_xz.out & m_xz.out





i_xz.out & m_xz.out





10. Contents of wsr.dat (wsr04.dat), 38s

```
Digit 1        10        20        30        40        50
  ** wsr.dat
  *        hm        trc        wb(um)   kfl(0,1)  kot       ity
          5.0        1.0          2.0         0      0         0
  *       wdx(um)    wdy(um)    dxy(um)     dz(um)
         14.0        0.0         0.01       0.01
  *       Lam(um)     th(deg)    fi(deg)    gm(deg)
          0.5       -45.0        0.0        90.0
  *       alx        aly        sx0(um)    sy0(um)
          0.2        1.0         2.0        0.0
  *       stx(um)    sty(um)    csx(um)    csy(um)
          0.0        0.0         0.0        0.0
  * km    *     Name  ko        an         ab         ak
     1         -SiO2   1     2.0000       0.00     0.0000
     2#          -Al   1     2.0000       0.00     0.0000   Digit60        70        80        90       100       110
  * kr         * kd   kt      ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)    xp
     1#           0    4       0.0       1.50       1.50      0.500       0.50       0.00       0.00     0.0
  * kf    km   kr kd   kt      ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)    xp        xq
     1#    1    0  0    1       0.0       1.00      1.000       0.50       0.50     -0.000       0.00     0.0       0.0
     2#    2    0  0    4       0.0       2.00       2.00       1.00       1.00      0.000       0.00     0.0       0.0
  * kb  kl  km  kp        tk    kf    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
     1   0   1   0      5.00     0    0
     2   0   0   0      5.00     0    0
```

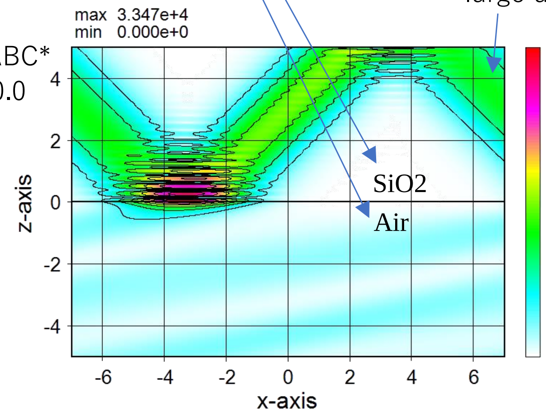
wb Absorbing boundary width (um). =0 is for no absorbing boundaries. The larger the value, the more non-reflective the boundaries are, but the amount of calculation increases .
kfl =0: Drawing without absorbing boundaries.
 =1: Drawing with absorbing boundaries.
kot Distributions such as intensity, absorption, and refractive index are output in a maximum of (kot+5) digits.
ity Definition of intensity distribution.
 =0 : magnitude of Poynting Vector,
 =1 : electric & magnetic fielf intensity,
 =2 : electric fielf intensity, =3 : magnetic fielf intensity.

The general RCWA method assumes periodic boundary conditions and no absorbing boundaries. The incident light source is also limited to uniformly distributed one. In wsr, both absorbing boundaries and distributed light sources can be set. When absorbing boundaries are set up, the problem of aliasing is eliminated, and the analysis space can be significantly reduced. On the other hand, since absorption is measured at the absorbing boundaries, it is not suitable to calculate transmittance and reflectance over the entire analysis area.

Memory consumption is small in layers of uniform refractive index, and it is automatically saved in wsr. However, for wb>0, the memory savings do not work because the refractive index distribution is not uniform due to the absorption of the boundaries (Compressed memory rate becomes 1.)

large aliasing

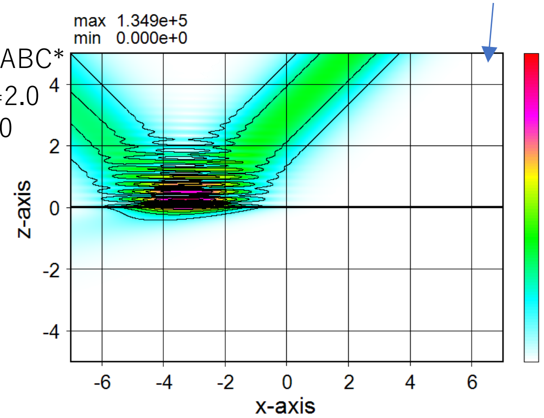
Without ABC*
wb=0.0
kfl=0



i_xz.out & m_xz.out

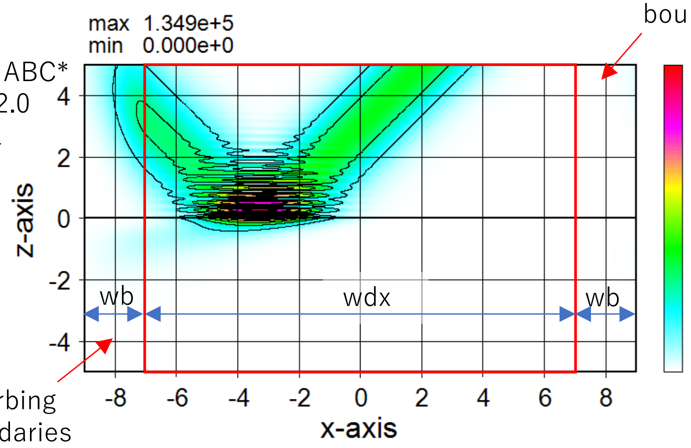
small aliasing

With ABC*
wb=2.0
kfl=0



absorbing boundaries

With ABC*
wb=2.0
kfl=1



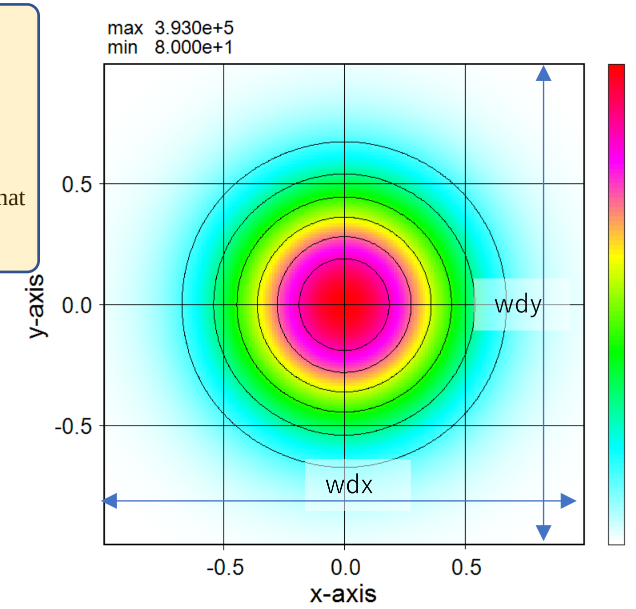
absorbing boundaries

(*) ABC=Absorbing Boundary Condition

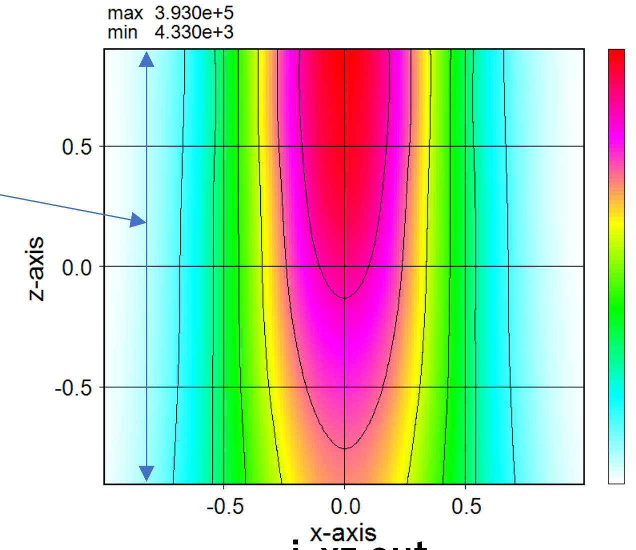
11. Contents of wsr.dat (wsr05.dat), 939s

```
Digit 1        10        20        30        40        50
** wsr.dat
*        hm       trc        wb(um)   kfl(0,1)  kot       ity
        5.0       1.0       0.5         0         0         0
*       wdx(um)   wdy(um)   dxy(um)    dz(um)
        2.0       2.0      0.01      0.01
*       Lam(um)   th(deg)   fi(deg)   gm(deg)
        0.5       0.0       0.0      90.0
*       alx       aly       sx0(um)   sy0(um)
        0.4       0.4       0.0       0.0
*       stx(um)   sty(um)   csx(um)   csy(um)
        0.0       0.0       0.0       0.0
* km   *     Name  ko       an        ab        ak
    1#      -SiO2   1    2.0000      0.00    0.0000
    2#        -Al   1    2.0000      0.00    0.0000   Digit60       70        80        90       100       110
* kr          * kd     kt   ps(deg)   px(um)   py(um)   wx(um)   wy(um)   sx(um)   sy(um)   xp
    1#           0      4       0.0     1.50     1.50    0.500     0.50     0.00     0.00    0.0
* kf    km    kr kd     kt   ps(deg)   px(um)   py(um)   wx(um)   wy(um)   sx(um)   sy(um)   xp        xq
    1#   1     0  0      1       0.0     1.00    1.000     0.50     0.50   -0.000     0.00    0.0       0.0
    2#   2     0  0      4       0.0     2.00     2.00     1.00     1.00    0.000     0.00    0.0       0.0
* kb  kl  km  kp        tk   kf    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
    1   0   0   0      0.60   0    0
    2   0   0   0      0.60   0    0
    3   0   0   0      0.60   0    0
```

wdx Analysis width in the x direction (um). wdx=0 becomes a 2-dimensional problem. The center of the width is the positional basis for the light source and structures. The larger the width, the larger the number of harmonics required.
wdx Analysis width in the y direction (um). wdy=0 becomes a 2-dimensional problem. The center of the width is the positional basis for the light source and structures. The larger the width, the larger the number of harmonics required.
dxy Grid interval in x/y direction (um). The actual interval is optimized to be close to that and displayed in wsr.out. The value should be less than 1/10 of the wavelength.
dz Grid interval in-z direction (um).



i_xy.out (1st in Wscnt)

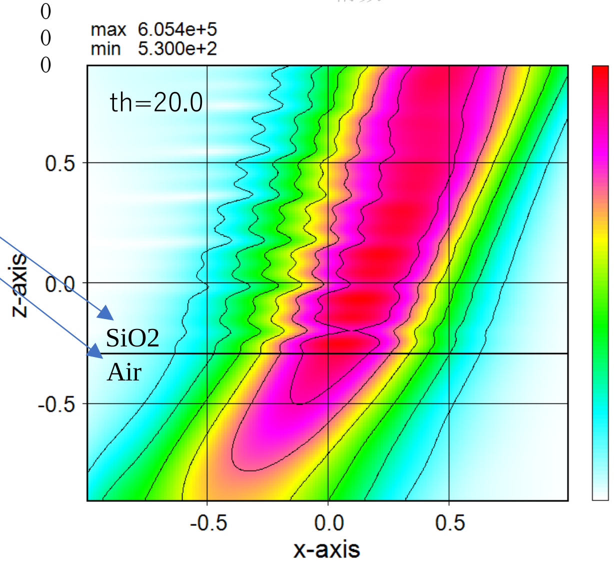


i_xz.out

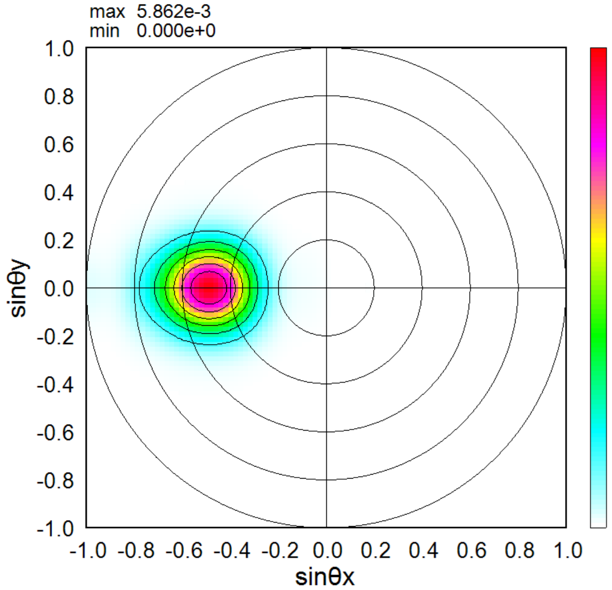
12. Contents of wsr.dat (wsr06.dat), 941s

```
Digit 1        10        20        30        40        50
** wsr.dat
*       hm        trc         wb(um)   kfl(0,1)  kot        ity
        5.0       1.0         0.5          0        0          0
*      wdx(um)   wdy(um)    dxy(um)    dz(um)
        2.0       2.0        0.01       0.01
*      Lam(um)    th(deg)    fi(deg)   gm(deg)
        0.5      -20.0        0.0       90.0
*      alx        aly        sx0(um)   sy0(um)
        0.4       0.4        0.5        0.0
*      stx(um)   sty(um)    csx(um)   csy(um)
        0.0       0.0        0.0        0.0
* km  *   Name  ko        an         ab        ak
   1      -SiO2  1      2.0000       0.00     0.0000
   2#       -Al  1      2.0000       0.00     0.0000    Digit60    70       80       90       100      110
* kr         * kd   kt      ps(deg)   px(um)   py(um)   wx(um)   wy(um)   sx(um)   sy(um)   xp
   1#           0    4      0.0       1.50     1.50     0.500    0.50     0.00     0.00     0.0
* kf   km   kr kd  kt      ps(deg)   px(um)   py(um)   wx(um)   wy(um)   sx(um)   sy(um)   xp       xq
   1#   1    0  0   1      0.0       1.00     1.000    0.50     0.50    -0.000    0.00     0.0      0.0
   2#   2    0  0   4      0.0       2.00     2.00     1.00     1.00     0.000    0.00     0.0      0.0
* kb   kl   km  kp       tk    kf   *    *    *    *    *  桁数 * 70 *  * 80 *  * 90 *  * 100 *  * 110 *
   1    0    1   0      0.60    0   0
   2    0    1   0      0.60    0   0
   3    0    0   0      0.60    0   0
```

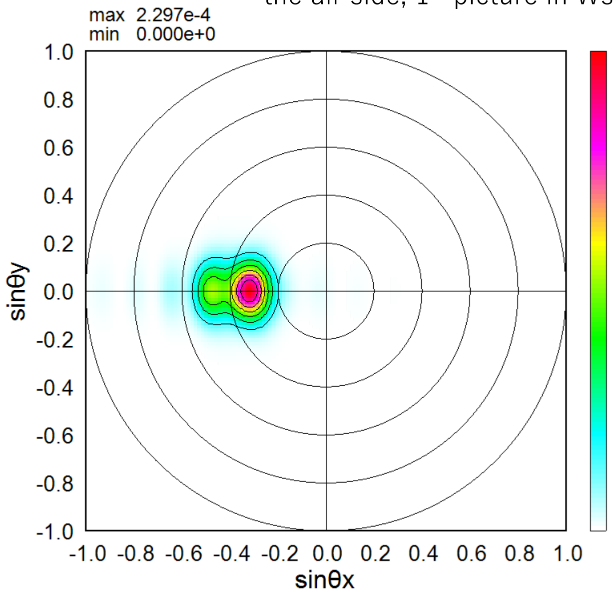
Lam	Wavelength (um).
th	Azimuth angle of incident light with z-axis (deg).
fi	Argument angle of incident light with x-axis in xy-plane (deg).
gm	Polarizing angle of light source that the electric field vector makes with the x-axis in xy plane (deg).



i_xz.out



i_far.out Far-field intensity distribution from the air side, 1st picture in Wscnt



i_far.out Far-field intensity distribution from SiO2 side, 2nd picture in Wscnt

13. Contents of wsr.dat (wsr07.dat), 828s

While conventional RCWA methods are limited to a uniformly distribution for incident light, in wsr, a distributed light source can be set.

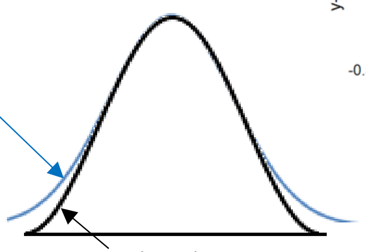
Any setting other than 1.0 will generate diffraction orders in the source light.

The full width at half-maximum is effectively larger because the outer edge intensity is lifted up compared to the cos intensity distribution. To match this width to that of the cos intensity distribution, a setting of 80% size is preferred.

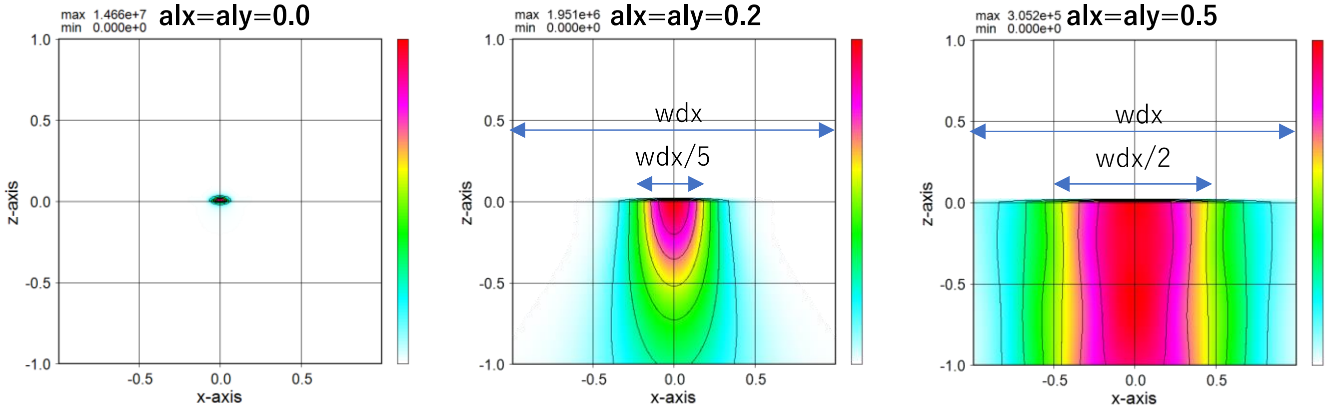
In the conventional RCWA method, the position of incident light is limited to the top surface. In wsr, it can be set at any desired position.

```
Digit 1       10        20        30        40        50
** wsr.dat
*       hm        trc        wb(um)   kfl(0,1)   kot          ity
        5.0       1.0       0.5          0        0            0
*       wdx(um)   wdy(um)   dxy(um)    dz(um)
        2.0       2.0       0.01       0.01
*       Lam(um)    th(deg)   fi(deg)    gm(deg)
        0.5       0.0       0.0        90.0
*       alx       aly       sx0(um)    sy0(um)
        0.5       0.5       0.0        0.0
*       stx(um)   sty(um)   csx(um)    csy(um)
        0.0       0.0       0.0        0.0
* km    *     Name   ko       an         ab        ak
   1#        -SiO2    1     2.0000      0.00    0.0000   Digit60    70        80        90       100       110
   2#          -Al    1     2.0000      0.00    0.0000
* kr         * kd    kt      ps(deg)    px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)    xp
   1#           0     4       0.0       1.50      1.50      0.500     0.50      0.00      0.00      0.0
* kf    km    kr kd   kt      ps(deg)    px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)    xp        xq
   1#    1     0  0    1       0.0       1.00      1.000     0.50      0.50     -0.000     0.00      0.0       0.0
   2#    2     0  0    4       0.0       2.00      2.00      1.00      1.00      0.000     0.00      0.0       0.0
* kb   kl   km   kp       tk     kf     *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
   1    1    0    0      1.00     0     0
   2    0    0    0      1.00     0     0
```

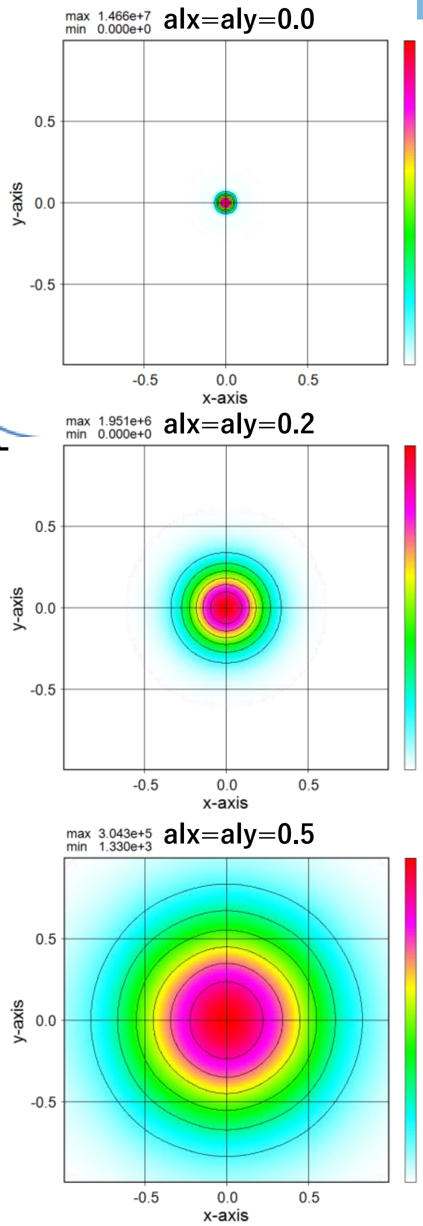
alx Light source spread in x-direction (um).
 =1.0 : uniform distribution.
 =0.0 : Minimum x-width.
 =0-1 : full width half maximum in x direction = wdx*alx.
aly Light source spread in y-direction (um).
 =1.0 : uniform distribution.
 =0.0 : Minimum y-width.
 =0-1 : full width half maximum in y direction = wdx*alx.
sx0 Shift length of light source center in x-direction (um).
sy0 Shift length of light source center in y-direction (um).



cos distribution



i_xz.out

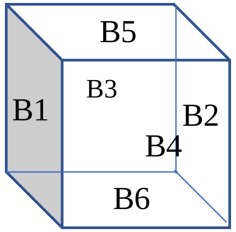


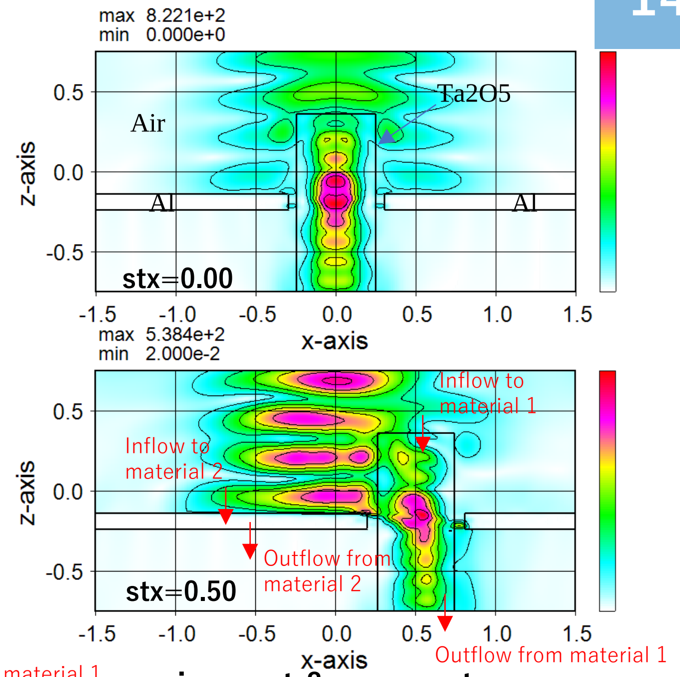
i_xy.out

Intensity distribution at the source position, 2nd picture in Wscnt

14. Contents of wsr.dat (wsr08.dat), 0.7s

When up/down is set to a reversal mode in Wscnt, "up" is correspond to -z side and "down" is to +z side.





i_xz.out & m_xz.out

```
Digit 1      10         20         30         40         50
   ** wsr.dat
   *       hm         trc         wb(um)     kfl(0,1)   kot         ity
          5.0         1.0         0.0          0          0           0
   *      wdx(um)     wdy(um)     dxy(um)    dz(um)
          3.0         0.0         0.01       0.01
   *      Lam(um)     th(deg)     fi(deg)    gm(deg)
         0.94         0.0         0.0        0.0
   *      alx         aly         sx0(um)    sy0(um)
          0.3         0.3         0.0        0.0
   *      stx(um)     sty(um)     csx(um)    csy(um)
          0.5         0.0         0.0        0.0
   * km   *    Name   ko       an         ab         ak
      1       Ta2O5    1     1.0000     0.00     0.0000
      2         -Al    1     1.4500     0.00     0.0000   Digit60    70         80         90        100        110
   * kr          * kd   kt     ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)     xp
      1#            0    4     0.0        1.50       1.50      0.500      0.50       0.00       0.00       0.0
   * kf    km    kr kd  kt     ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)     xp         xq
      1     1     0  0   2     0.0        0.00       0.00       0.50       0.50      0.000       0.00       0.0        0.0
      2     2     0  0  -2     0.0        0.00       0.00       0.60       0.60      0.000       0.00       1.0        0.0
   * kb   kl   km   kp        tk       kf     *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
      1    0    0    0      0.40       0     0
      2    0    0    0      0.50       1     0
      3    0    0    0      0.10       1     2
      4    0    0    0      0.50       1     0
```

stx Shift length of overall structure center in x-direction (um). Not applicable for light source position.
sty Shift length of overall structure center in y-direction (um). Not applicable for light source position.
csx Cross sectional position of graphics in x-direction (um).
csy Cross sectional position of graphics in y-direction (um).

Harmonics number(x/y-axis)

```
*** Copyright (c) WS-soft. All rights reserved. Revised on 2022/01/01.  ***
    Analyzed range (x/y/z) =   3.00/   3.00/   1.50 (um)
    Grid size    (dx/dy/dz) = 0.0118/*******/ 0.0100(um), m= 8
    Harmonics factor hm/trc= 5.0/1.00,   Harmonics number (x/y)=  15/   0
    Matrix size (1D)=  31,    Truncation rate=1.000
 * Structural matrixes...
    L =  1 /   4   Homogeneous index layer        0.00sec
    L =  2 /   4   Mixed index layer              0.00sec
    L =  3 /   4   Mixed index layer              0.00sec
    L =  4 /   4   Mixed index layer              0.00sec
 * Compressed memory rates...
    L =  4 /   4   0.499935
    L =  3 /   4   0.499935
    L =  2 /   4   0.499935
    L =  1 /   4   0.257999
    Average        0.439451
```

Calculation of convolution matrix, structural matrix

Structural matrix of each layer

Compression ratio of memory at each layer

Memory consumption is small in layers of uniform refractive index, and it is automatically saved in wsr.

Total compression ratio of memory

Diffraction efficiency for reflection
Diffraction order in y-direction
Diffraction order in x-direction
Diffraction efficiency for transmission
Absorption efficiency
Efficiency for R + T
Efficiency for R + T + A

```
 * Diffractive power distributions...
   -15   0    0.00E+00  -9.67E-06   0.00E+00   0.00E+00   -9.67E-06
   -14   0    0.00E+00  -3.71E-05   0.00E+00   0.00E+00   -3.71E-05
                                        .  .  .
    15   0    0.00E+00   5.41E-05   0.00E+00   0.00E+00    5.41E-05
     m   n    Ref(-z)     Absp      Trn(+z)      R+T        R+A+T      Guided
   Total      0.617036   0.107291   0.275686   0.892723   1.000013   -0.000013
 * Intensity distributions...
    L =  1 /  4      0.06sec
    L =  2 /  4      0.06sec
    L =  3 /  4      0.01sec
    L =  4 /  4      0.06sec
```

Solution of eigenvalue problems and alignment of matrices

Total efficiency

Efficiency of lateral diffraction

Solution of wave equations and calculation of light distribution at each layer

outflow (-) and inflow (+) at boundaries of each material and their summation

Excerpt of wsr.out

Layer number
Divergence/absorption efficiency at material 0
Efficiency at material 1
Efficiency at material 2

```
 * Divergence(-)/absorptions(+) at Materials ...
                 an(00)      an(01)      an(02)
   L =  1 /  4   0.249491    0.000000    0.000000
   L =  2 /  4  -0.221179    0.276730    0.000000
   L =  3 /  4   0.007123    0.004472    0.064428
   L =  4 /  4  -0.004732   -0.269043    0.000000
   Total         0.030703    0.012159    0.064428
 * Flows from analytic boundaries(out:-, in:+)...
        -x          +x          -y          +y          -z          +z        Total     Absorbed
    0.035934   -0.035934    0.000000    0.000000   -0.275673   -0.617036   -0.892709    0.107291
 * Material boundary flows  (out:-, in:+) and divergence(-)/absorptions(+)...
        -x          +x          -y          +y          -z          +z        Total
    0.180900   -0.233539    0.000000    0.000000   -0.301519    0.384862    0.030703,  an(00)= 1.00000   ak(00)= 0.00000
    0.194673   -0.130439    0.000000    0.000000   -0.185548    0.133472    0.012159,  an(01)= 2.10205   ak(01)= 0.00000   Ta2O5
    0.003698   -0.015293    0.000000    0.000000   -0.001898    0.077921    0.064428,  an(02)= 1.73131   ak(02)= 8.59626   Al
 Transmitted   Reflected   Absorbed    Rest      01/lower-in  upper-out   absorbed   02/lower-in  upper-out   absorbed
 2.7567E-01   6.1704E-01  1.0729E-01  1.5149E-08  1.3347E-01  1.8555E-01  1.2159E-02  7.7921E-02  1.8981E-03  6.4428E-02
```

Total efficiency for each material

outflow (-) and inflow (+) at analysis boundaries

Absorbing efficiency inside analysis boundaries

Material No./Optical index   Name

Total light- amount
Light-amount for material 1
Light-amount for material 2

Output to wsr1.out

15. Contents of wsr.dat (wsr09.dat), 22s

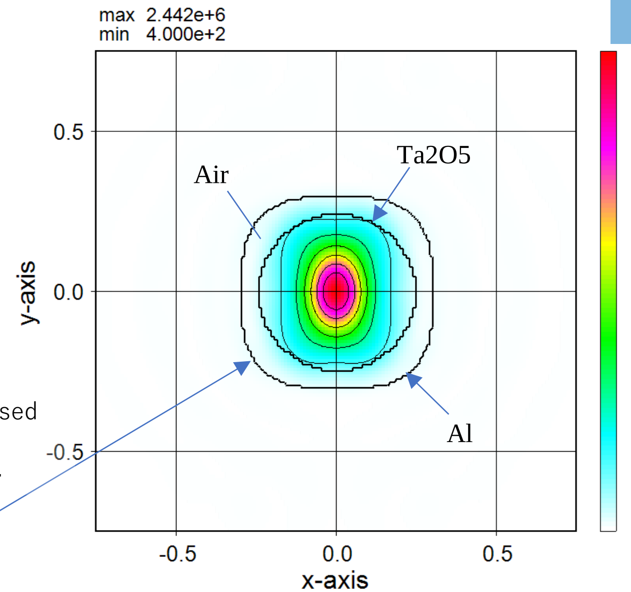
```
Digit 1       10         20         30         40         50
** wsr.dat
*        hm         trc         wb(um)    kfl(0,1)  kot         ity
        5.0         1.0         0.5          0         0           0
*       wdx(um)     wdy(um)     dxy(um)     dz(um)
        1.5         1.5        0.01       0.01
*       Lam(um)      th(deg)     fi(deg)    gm(deg)
       0.94         0.0         0.0        0.0
*       alx         aly         sx0(um)    sy0(um)
        0.3         0.3         0.0        0.0
*       stx(um)     sty(um)     csx(um)    csy(um)
        0.0         0.0         0.0        0.0
* km   *    Name ko          an         ab          ak
   1       Ta205  1      1.0000       0.00      0.0000
   2        -Al   1      2.0000       0.00      0.0000   Digit60      70         80         90        100        110
* kr          * kd   kt      ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)       xp
   1#            0    4         0.0      1.50       1.50      0.500       0.50       0.00       0.00       0.0
* kf   km   kr kd   kt      ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)       xp          xq
   1    1    0  0    2         0.0      0.00       0.00       0.50       0.50      0.000       0.00       0.0         0.0
   2    2    0  0   -2         0.0      0.00       0.00       0.60       0.60      0.000       0.00       1.0         0.0
* kb   kl   km   kp        tk    kf     *     *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
   1    0    0    0      0.40     0     0
   2    0    0    0      0.50     1     0
   3    0    0    0      0.10     1     2
   4    0    0    0      0.50     1     0
```

Calculated as external data

If unregistered, only up to two lines can be read.

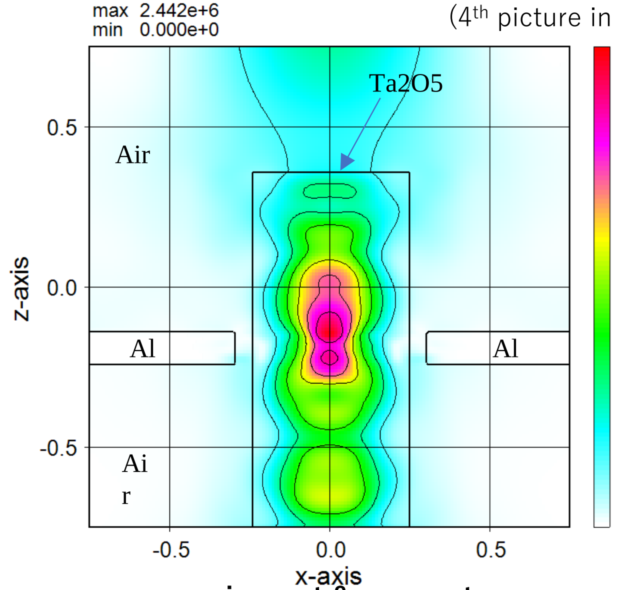
Calculated as internal data

Corner R is expressed by setting elliptic exponent index xp.



i_xy.out & m_xy.out

(4th picture in Wscnt)



i_xz.out & m_xz.out

(3rd picture in Wscnt)

km designation field (for optical materials)

The first 4 digits are serial line numbers, up to 200 lines can be input. Name Material name (within 8 digits) SiO2, Ag, Al, Au, Be, Cr, Cu, Ni, Pd, Pt, Ti, W have internal data. For others, by entering the wavelength, refractive index, and extinction coefficient in the file of nk.dat as external data, the refractive index and extinction coefficient are automatically interpolated. If no data exists in nk.dat, the values defined by the right-side parameters of 'an' are given priority. nk.dat should be created by each user and stored in the same folder as wsb.exe.

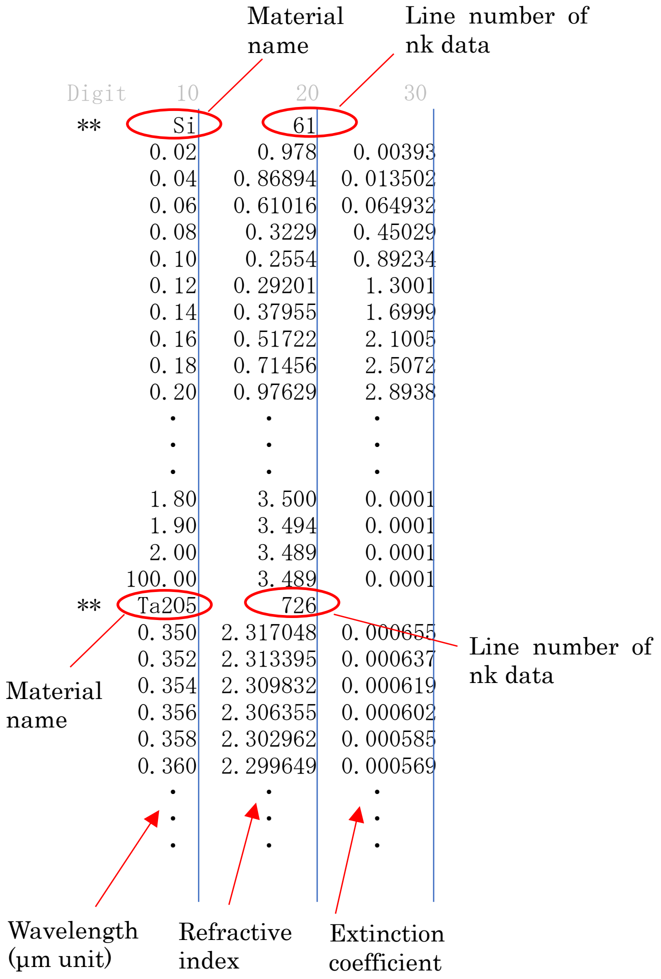
ko Whether to output detected light amount to wsb1.out or not.
=0 : not output, =1 : output.

an Refractive index.

ab Abbe number, if =0, no dispersion (fixed to refractive index).

ak Extinction coefficient.

16. Contents of nk.dat



Excerpt from nk.dat

Numerical Data Input Rule

- After entering the delimiter mark (**) on the first line of the numerical data, write the material name (8 columns) and the number of lines of nk.dat (10 columns).
- Input numbers are half-width (Spaces should be half-width and Tab codes are not allowed).
- The right edge of the input digit must be aligned with a vertical line in 10-digit increments.
- Input numbers should be spaced by at least one half-width space.

The material data can be created by overlaying the actual measured values or literature values, etc. in the format shown above. The file name should be "nk.dat" and must be stored in the folder where wsr.exe is located. However, the material name must be other than -SiO2, -Ag, -Al, -Au, -Be, -Cr, -Cu, -Ni, -Pd, -Pt, -Ti, -W which are defined in internal materials. If there are duplicate material names, the first data takes priority.

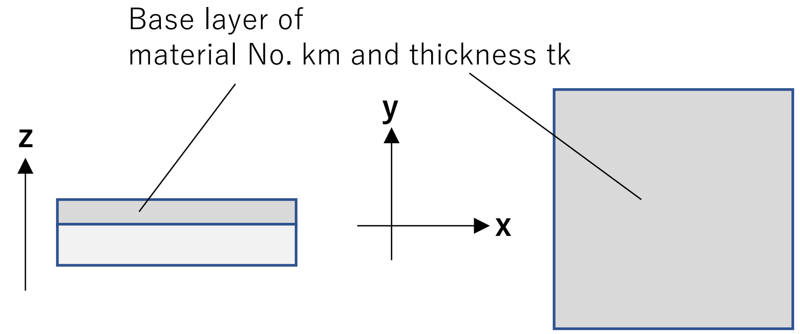
References

https://refractiveindex.info/?shelf=main&book=Ta2O5&page=Bright-amorphous

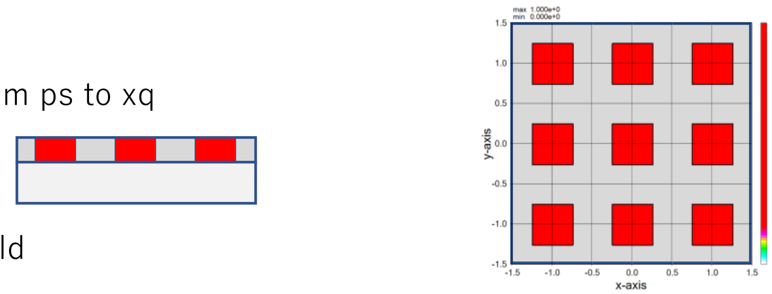
https://www.filmetricsinc.jp/refractive-index-database/Ta2O5

17. Procedure for defining optical structures

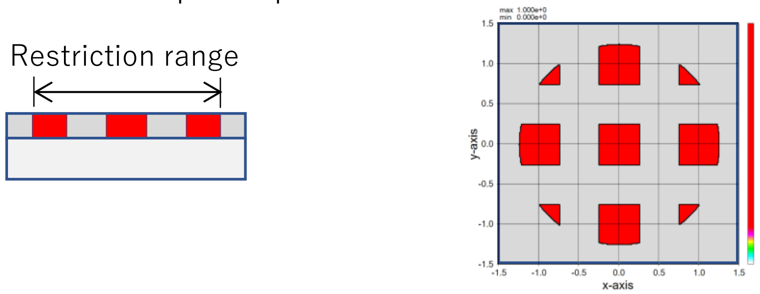
① Definition of a Base layer
1. setting km and tk
2. entering kf for reference



② Definition of periodic structures
on a Base layer at Kf specification field
1. setting km,kd,and kt
2. definition of structures by setting parameters from ps to xq
3. entering kr for reference



③ Restriction of periodic structures at Kr specified field
1. setting kd and kt
2. definition of the restriction shape by setting parameters from ps to xp




```
** wsr.dat
*        hm        trc        wb(um)    kfl(0,1)   kot        ity
         5.0       1.0        0.0          0         0          0
*        wdx(um)   wdy(um)    dxy(um)   dz(um)
         3.0       3.0        0.01      0.01
*        Lam(um)    th(deg)   fi(deg)   gm(deg)
        0.94       0.0        0.0       0.0
*        alx       aly        sx0(um)   sy0(um)
         0.3       0.3        0.0       0.0
*        stx(um)   sty(um)    csx(um)   csy(um)
         0.0       0.0        0.0       0.0
* km   *     Name  ko        an        ab        ak
   1        -SiO2   1    2.0000      0.00    0.0000
   2#         -Al   1    2.0000      0.00    0.0000
* kr          * kd   kt      ps(deg)   px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)    xp
   1            0    2       0.0       0.00      0.00      2.50      2.50      0.00      0.00      0.0
* kf   km   kr kd   kt      ps(deg)   px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)    xp        xq
   1    1    1  0    1       0.0       1.00      1.000     0.50      0.50     -0.000     0.00      0.0       0.0
   2#   2    0  0    4       0.0       2.00      2.00      1.00      1.00      0.000     0.00      0.0       0.0
* kb  kl  km  kp        tk    kf    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
   1   0   0   0      0.60     1    0
```

Kr field ③
Kf field ②
① Base layer

18. Contents of wsr.dat (wsr10.dat), 85s

```
Digit 1        10        20        30        40        50
      ** wsr.dat
      *        hm       trc    wb(um)  kfl(0,1)   kot         ity
              5.0       1.0       0.0        0      0           0
      *    wdx(um)   wdy(um)   dxy(um)    dz(um)
              3.0       3.0      0.01      0.01
      *    Lam(um)   th(deg)   fi(deg)   gm(deg)
             0.94       0.0       0.0       0.0
      *       alx       aly   sx0(um)   sy0(um)
              0.3       0.3       0.0       0.0
      *    stx(um)   sty(um)   csx(um)   csy(um)
              0.0       0.0       0.0       0.0
      * km   *   Name  ko        an        ab        ak
         1      -SiO2   1    2.0000      0.00    0.0000
         2#       -Al   1    2.0000      0.00    0.0000  Digit60    70        80        90       100       110
      * kr         * kd   kt   ps(deg)    px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)    xp
         1#           0    2       0.0      0.00      0.00      2.50      2.50      0.00      0.00    0.0
      * kf  km  kr  kd   kt   ps(deg)    px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)    xp        xq
         1   1   0   0    2       0.0      1.00     1.000      0.50      0.50    -0.000      0.00    0.0       0.0
         2#  2   0   0    4       0.0      2.00      2.00      1.00      1.00     0.000      0.00    0.0       0.0
      * kb  kl  km  kp        tk   kf   *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
         1   0   0   0      0.60    1   0
```

See the pages that follow for relationship with figures.

Referred

ps Rotation angle of all structures around the region center (deg).
px Structure period in x-direction (um). When =0, it is an isolated pattern.
py Structure period in y-direction (um). When =0, it is an isolated pattern.
wx Structure width in y-direction (um).
wy Structure width in y-direction (um).
sx Shift length of the structure center in x-direction (um).
sy Shift length of the structure center in y-direction (um).
xp Elliptic exponent index for kt=2. Lattice duty ratio for kt=10 to 17.
xq Starting point of lattice for kt=10 to 17.

Defined inside periodic circles

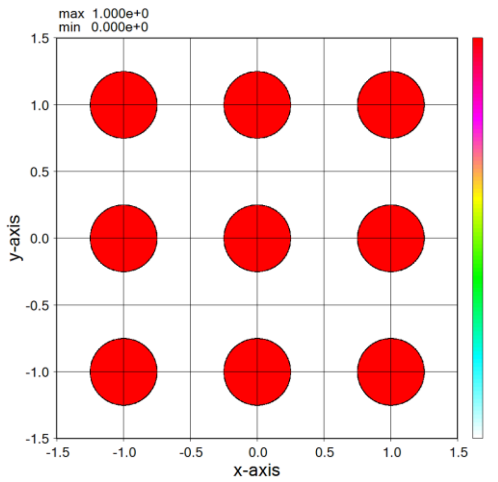
Defined outside periodic circles

kf designation field (for foreground structures)

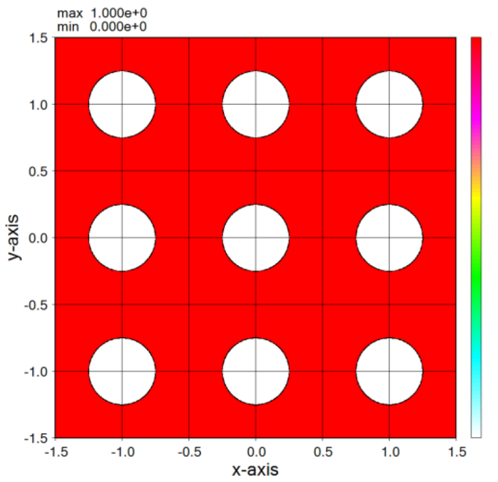
The first 4 digits are serial line numbers, up to 9999 lines can be input.
km Construction material number referred in km designation field. km=0 means vacuum (n=1.0).
kr Restriction shape number referred in kr designation field. kr=0 means restriction free.
kd How to input shape data of structures. =0: by internal definition. =1: by external data using sub.dat.
Applied to all except for wx and wy, sub.dat can be input up to 400 types (up to 1000 lines for each type).
kt Selection of shape type. (-kt shows an inverted shape for kt.)
When kd=1, kt=Pattern No. in sub.dat.
When kd=0,
kt=0 No area definition.
=1 Rectangular areas of width wx*wy centered on a square grid position of period px*py.
=2 Elliptic shape of width wx*wy and elliptic index xp centered on a square grid position of period px*py,
where xp = -2.0 to -1.0 for star, = -1.0 for diamond, = 0.0 for ellipse, > 0.0 for square.
=3 Hexagons shape (top/bottom vertex angles) of width wx*wy centered on a square grid position of period px*py.
=4 Hexagon shape (left/right vertex angles) of width wx*wy centered on a square grid position of period px*py.
=5 Diamond shape of width wx*wy centered on a square grid position of period px*py.
=6 Right-angled triangular shape (diagonal 1st quadrant) of width wx*wy centered on a square grid position of period px*py.
=7 Right-angled triangular shape (diagonal 2nd quadrant) of width wx*wy centered on a square grid position of period px*py.
=8 Right-angled triangular shape (diagonal 3rd quadrant) of width wx*wy centered on a square grid position of period px*py.
=9 Right-angled triangular shape (diagonal 4th quadrant) of width wx*wy centered on a square grid position of period px*py.

=10 Linear lattice of period wx, angle wy, duty ratio xp, starting point xq included in each square grid of period px*py.
=11 Concentrically elliptic lattice of period wx, angle wy, duty ratio xp, starting point xq included in each square px*py of period px*py.
=12 Concentrically dodecagonal lattice of period wx, angle wy, duty ratio xp, starting point xq included in each square grid of period px*py.
=13 15-degrees-rotated lattice for kt=12.
=14 Concentrically 18-corner polygonal lattice of period wx, angle wy, duty ratio xp, starting point xq included in each square grid of period px*py.
=15 10-degrees-rotated lattice for kt=14.
=16 Concentrically hexagonal lattice of period wx, angle wy, duty ratio xp, starting point xq included in each square grid of period px*py.
=17 30-degrees-rotated lattice for kt=16.

kt=2



kt=-2



m_xy.out

19. Contents of wsr.dat (wsr11.dat), 85s

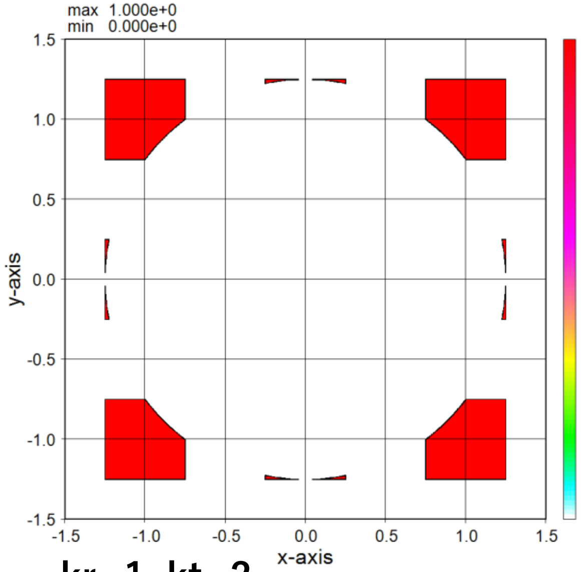
```
Digit 1        10         20         30         40         50
** wsr.dat
*        hm         trc          wb(um)     kfl(0,1)   kot         ity
         5.0        1.0          0.0        0          0           0
*        wdx(um)    wdy(um)      dxy(um)    dz(um)
         3.0        3.0          0.01       0.01
*        Lam(um)    th(deg)      fi(deg)    gm(deg)
         0.94       0.0          0.0        0.0
*        alx        aly          sx0(um)    sy0(um)
         0.3        0.3          0.0        0.0
*        stx(um)    sty(um)      csx(um)    csy(um)
         0.0        0.0          0.0        0.0
* km   *   Name  ko     an        ab       ak
    1     -SiO2   1   2.0000    0.00    0.0000
   2#       -Al   1   2.0000    0.00    0.0000   Digit60    70      80      90      100     110
* kr          * kd  kt  ps(deg)  px(um)  py(um)  wx(um)  wy(um)  sx(um)  sy(um)  xp
    1            0   2  0.0      0.00    0.00    2.50    2.50    0.00    0.00    0.0
* kf   km  kr  kd  kt   ps(deg)  px(um)  py(um)  wx(um)  wy(um)  sx(um)  sy(um)  xp   xq
    1   1   1   0   1   0.0      1.00    1.000   0.50    0.50    -0.000  0.00    0.0  0.0
   2#   2   0   0   4   0.0      2.00    2.00    1.00    1.00    0.000   0.00    0.0  0.0
* kb  kl  km  kp    tk   kf   *  *  *  *  *  *  *  *  *  *  *  *  *  *  *  *
    1   0   0   0   0.60  1   0
```

Referred

ps Rotation angle of all structures around the region center (deg).
px Structure period in x-direction (um). When =0, it is an isolated pattern.
py Structure period in y-direction (um). When =0, it is an isolated pattern.
wx Structure width in y-direction (um).
wy Structure width in y-direction (um).
sx Shift length of the structure center in x-direction (um).
sy Shift length of the structure center in y-direction (um).
xp Elliptic exponent index for kt=2. Lattice duty ratio for kt=10 to 17.

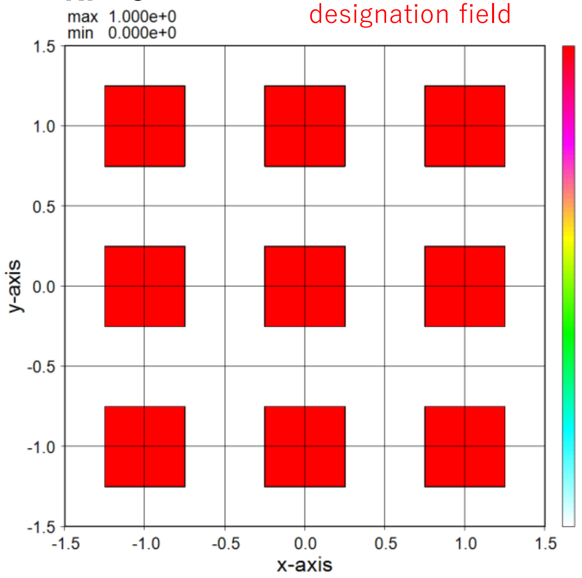
limited outside a circle by setting kr designation field

kr=1 kt=-2

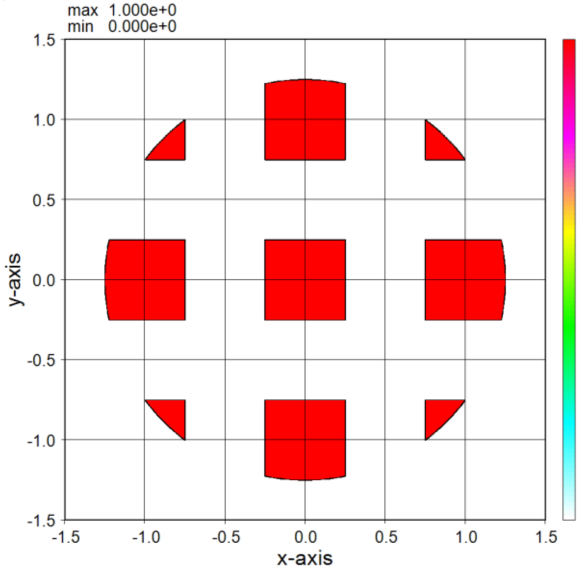


limited inside a circle by setting kr designation field

kr=0



kr=1 kt=2



m_xy.out

kr designation field (for restricting shapes)
The first 4 digits are serial line numbers, up to 1000 lines can be input.
kd How to input shape data of structures. =0: by internal definition. =1: by external data using sub.dat.
Applied to all except for wx and wy, sub.dat can be input up to 400 types (up to 1000 lines for each type).
kt Selection of shape type. (-kt shows an inverted shape for kt.)
When kd=1, kt=Pattern No. in sub.dat. When kd=0, kt=0 No area restriction.
=1 Restricted by rectangular areas of width wx*wy centered on a square grid position of period px*py.
=2 Restricted by elliptic shape of width wx*wy and elliptic index xp centered on a square grid position of period px*py, where xp = -2.0 to -1.0 for star, = -1.0 for diamond, = 0.0 for ellipse, > 0.0 for square.
=3 Restricted by hexagons shape (top/bottom vertex angles) of width wx*wy centered on a square grid position of period px*py.
=4 Restricted by hexagon shape (left/right vertex angles) of width wx*wy centered on a square grid position of period px*py.
=5 Restricted by diamond shape of width wx*wy centered on a square grid position of period px*py.
=6 Restricted by a right-angled triangular shape (diagonal fist quadrant) of width wx*wy centered on a square grid position of period px*py.
=7 Restricted by a right-angled triangular shape (diagonal second quadrant) of width wx*wy centered on a square grid position of period px*py.
=8 Restricted by a right-angled triangular shape (diagonal third quadrant) of width wx*wy centered on a square grid position of period px*py.
=9 Restricted by a right-angled triangular shape (diagonal fourth quadrant) of width wx*wy centered on a square grid position of period px*py.

20. Contents of wsr.dat (wsr12.dat), 1s

1	0	0	0	0.30	0	0
2	0	2	0	0.30	0	0
3	0	1	0	0.11180	0	0
4	0	2	0	0.16268	0	0
5	0	1	0	0.11180	0	0
6	0	2	0	0.16268	0	0
7	0	1	0	0.11180	0	0
8	0	2	0	0.16268	0	0
9	0	1	0	0.67082	0	0
10	0	2	0	0.16268	0	0
11	0	1	0	0.11180	0	0
12	0	2	0	0.16268	0	0
13	0	1	0	0.11180	0	0
14	0	2	0	0.16268	0	0
15	0	1	0	0.11180	0	0
16	0	2	0	0.16268	0	0
17	0	1	0	0.11180	0	0
18	0	2	0	0.16268	0	0
19	0	1	0	0.11180	0	0
20	0	2	0	0.16268	0	0
21	0	1	0	0.11180	0	0
22	0	2	0	0.16268	0	0
23	0	1	0	0.11180	0	0
24	0	2	0	0.16268	0	0
25	0	1	0	0.67082	0	0
26	0	2	0	0.16268	0	0
27	0	1	0	0.11180	0	0
28	0	2	0	0.16268	0	0
29	0	1	0	0.11180	0	0
30	0	2	0	0.16268	0	0
31	0	1	0	0.11180	0	0
32	0	2	0	0.16268	0	0
33	0	1	0	0.11180	0	0
34	0	2	0	0.16268	0	0
35	0	1	0	0.11180	0	0
36	0	2	0	0.16268	0	0
37	0	1	0	0.11180	0	0
38	0	2	0	0.16268	0	0
39	0	1	0	0.11180	0	0
40	0	2	0	0.16268	0	0
41	0	1	0	0.67082	0	0
42	0	2	0	0.16268	0	0
43	0	1	0	0.11180	0	0
44	0	2	0	0.16268	0	0
45	0	1	0	0.11180	0	0
46	0	2	0	0.16268	0	0
47	0	1	0	0.11180	0	0
48	0	2	0	0.30	0	0
49	0	0	0	0.30	0	0

10nm bandpass filter structure centered at 940nm

```
Digit 1        10        20        30        40        50
** wsr.dat
*        hm         trc          wb(um)   kfl(0,1)  kot         ity
        5.0         2.0         0.0          0         0          0
*       wdx(um)     wdy(um)     dxy(um)     dz(um)
        1.0         0.0        0.01        0.01
*       Lam(um)      th(deg)     fi(deg)     gm(deg)
       0.94         0.0         0.0         0.0
*       alx         aly         sx0(um)     sy0(um)
        1.0         1.0         0.0         0.0
*       stx(um)     sty(um)     csx(um)     csy(um)
        0.0         0.0         0.0         0.0
* km   *      Name  ko          an          ab          ak
    1        Ta2O5   1     2.11000        0.00       0.000
    2        -SiO2   1      1.0000        0.00      0.0000 Digit60   70        80        90        100       110
* kr           * kd   kt      ps(deg)     px(um)      py(um)      wx(um)      wy(um)      sx(um)      sy(um)      xp
    1#            0    2         0.0        0.00        0.00        2.50        2.50        0.00        0.00       0.0
* kf     km    kr kd   kt      ps(deg)     px(um)      py(um)      wx(um)      wy(um)      sx(um)      sy(um)      xp          xq
    1#    1     0  0    1         0.0        1.00       1.000        0.50        0.50      -0.000        0.00       0.0         0.0
    2#    2     0  0    4         0.0        2.00        2.00        1.00        1.00       0.000        0.00       0.0         0.0
* kb    kl    km   kp          tk    kf    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
    1    0     0    0        0.30     0    0
    2    0     2    0        0.30     0    0
    3    0     1    0     0.11180     0    0
    4    0     2    0     0.16268     0    0
      .    .    .
   47    0     1    0     0.11180     0    0
   48    0     2    0        0.30     0    0
   49    0     0    0        0.30     0    0
```

Light source position at top line

-z

Propagation direction cos(th)>0

+z

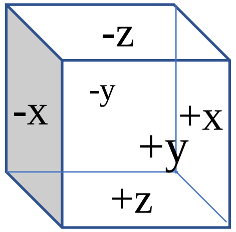
Insert a blank line beginning with "c" at the breakpoint to abort reading

Base layers

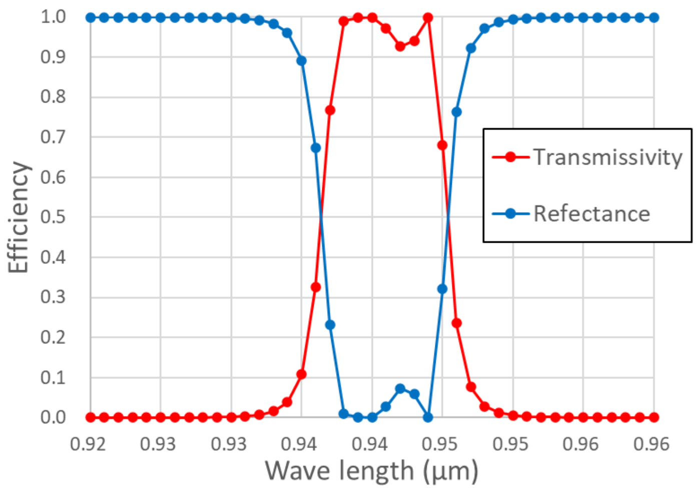
Up to 10000 lines can be input as far as the last line or the line starting from "c" appears. Optical constants above the top layer or below the bottom layer is the same ones as the top or the bottom layer, respectively, and then no boundary reflections from there.

- kl =1: light source position. If all of kl are 0, the –z-side surface of the first layer for cos(th)>0, or the +z-side surface of the last layer for cos(th)<0 is the light source position.
- km Construction material number referred in km designation field. km=0 means vacuum (n=1.0).
- kp Not operated (operated in wsb).
- tk Layer thickness (um)
- kf =0: No reference
  >0: Structure shape number referred in kf designation field. The referred shape structures are overwritten on the layer. This numbers are represented by four digits, up to 100 set per line.

Since the alignment of the structural layers is inverted on the z-axis and light propagation is also from –z to +z direction, it is easy to see when pictures displayed in Wscnt are vertically inverted to align a direction.



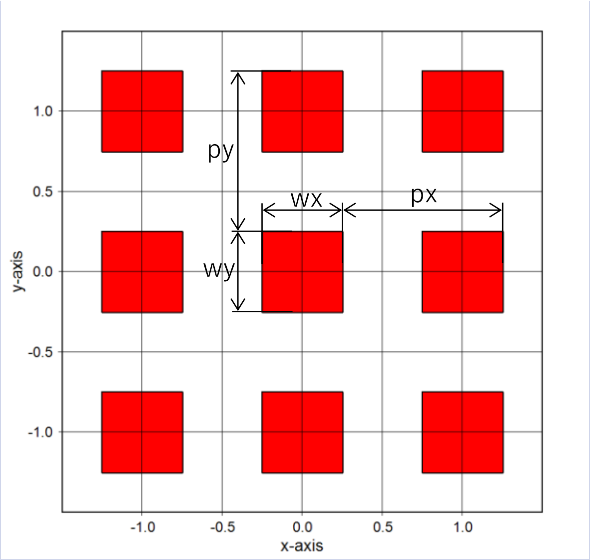
If "U/D_reverse" is checked in wscnt, B5/B6 is reversed as above.



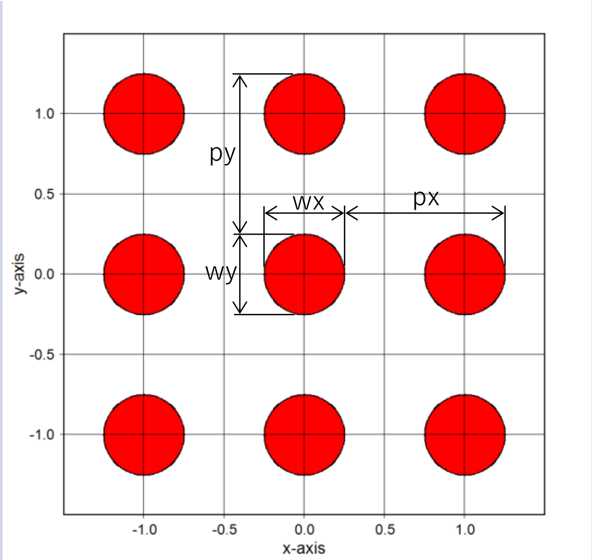
Result of wsr1.out

21. Relationships (1) between kt and structures for kd=0

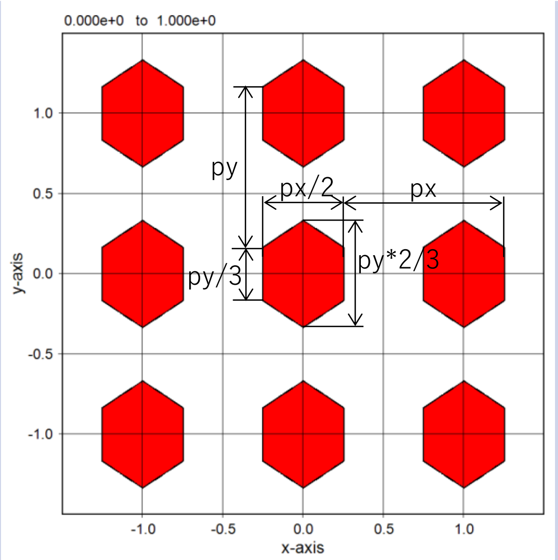
kt=1



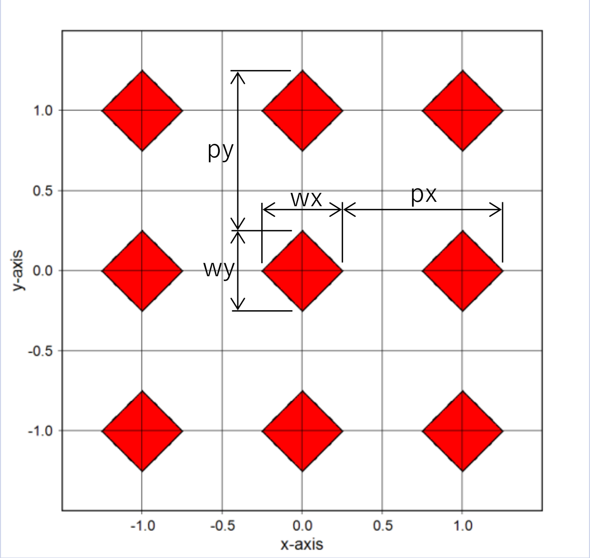
kt=2



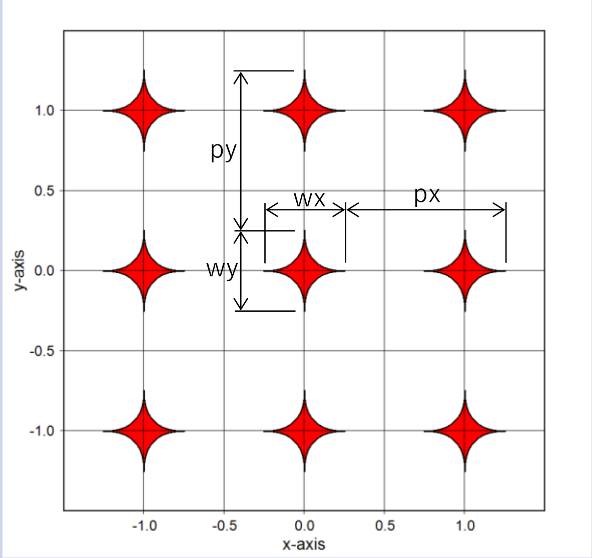
kt=3



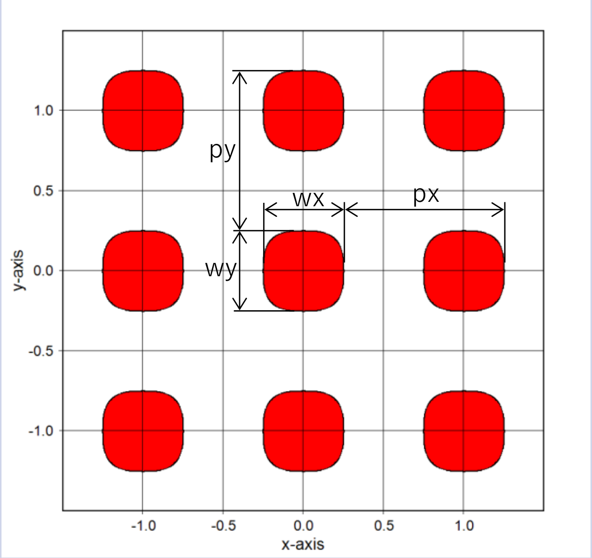
kt=2,xp=-1.0



kt=2,xp=-1.5

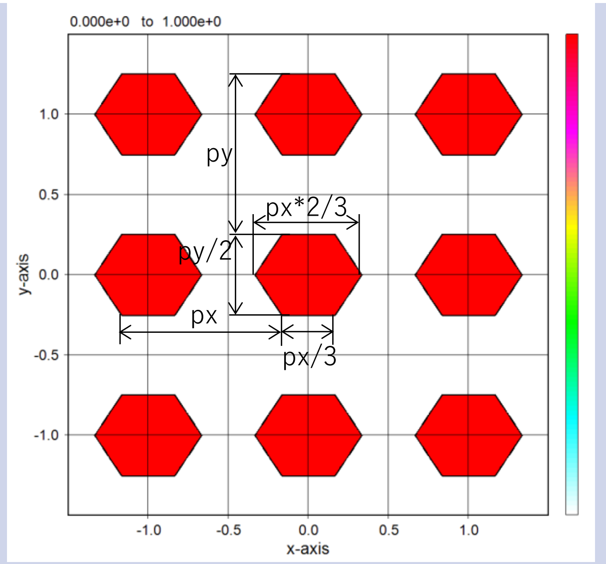


kt=2,xp=1.0

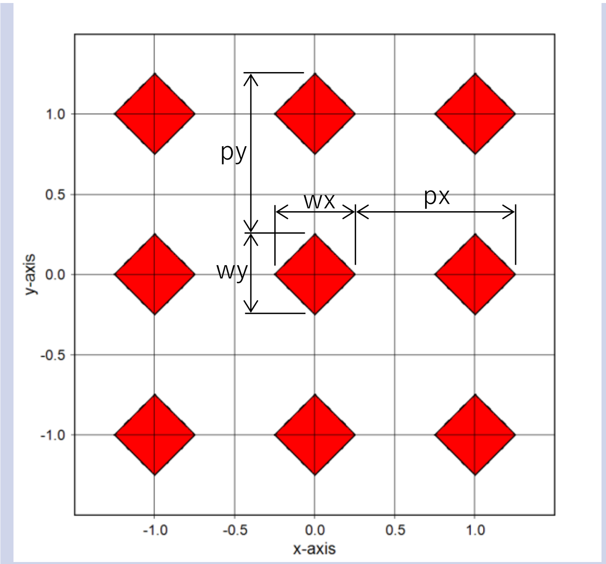


22. Relationships (2) between kt and structures for kd=0

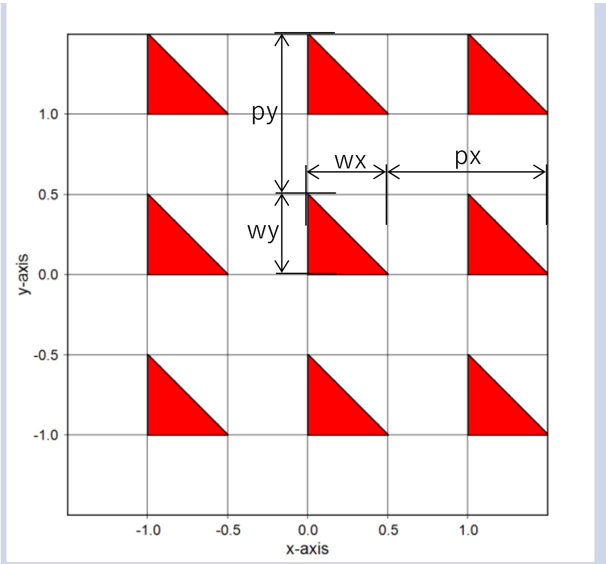
kt=4



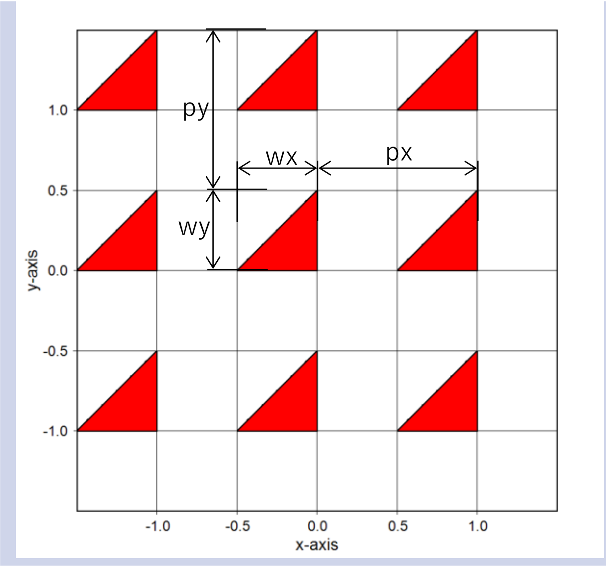
kt=5



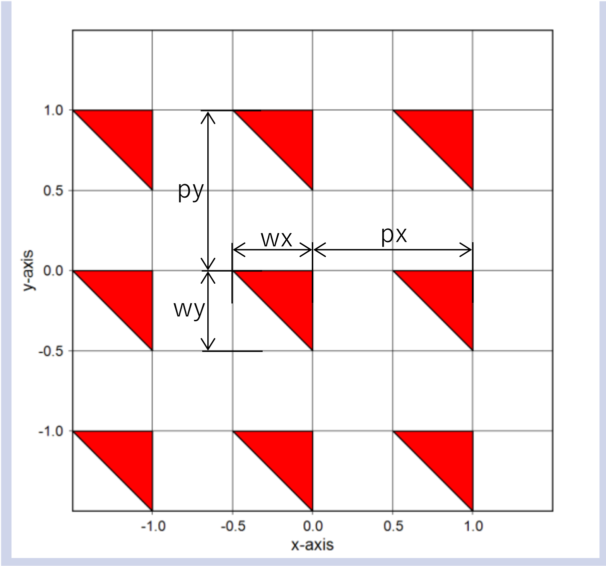
kt=6



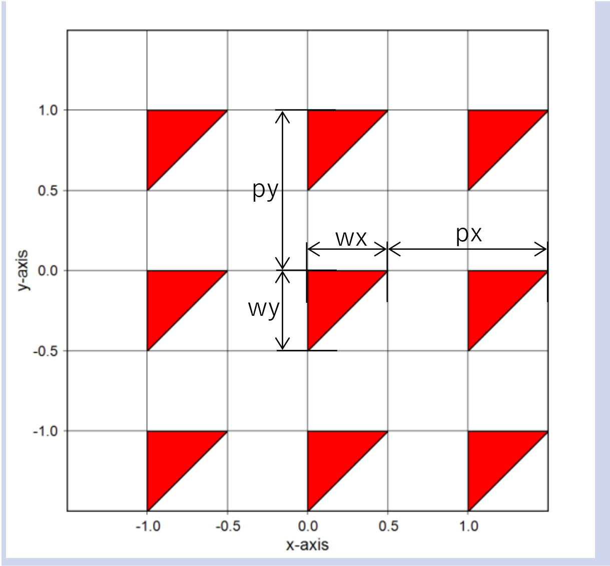
kt=7



kt=8

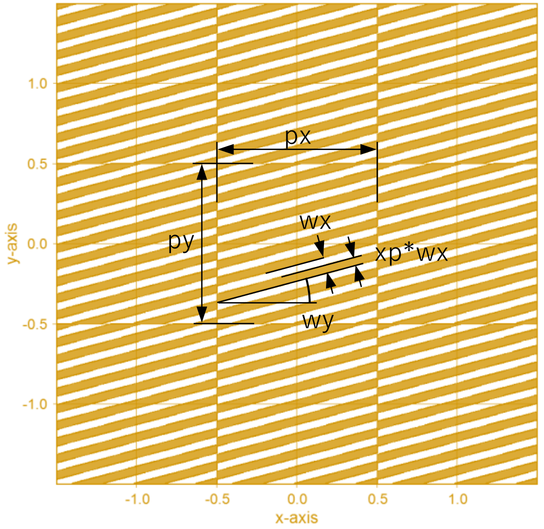


kt=9

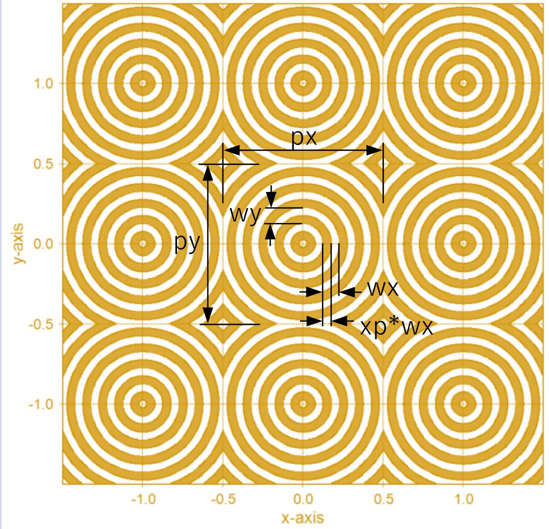


23. Relationships (3) between kt and structures for kd=0

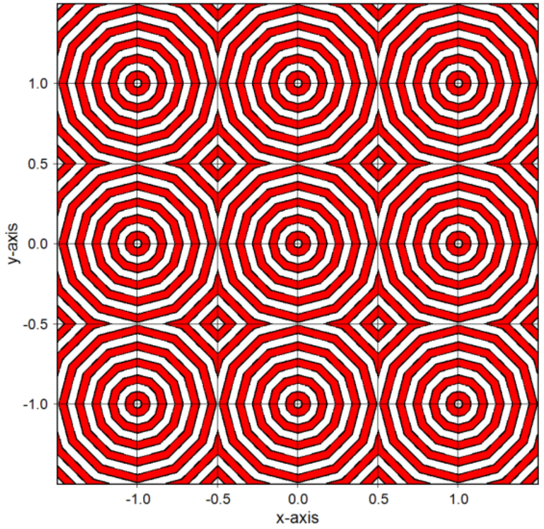
kt=10



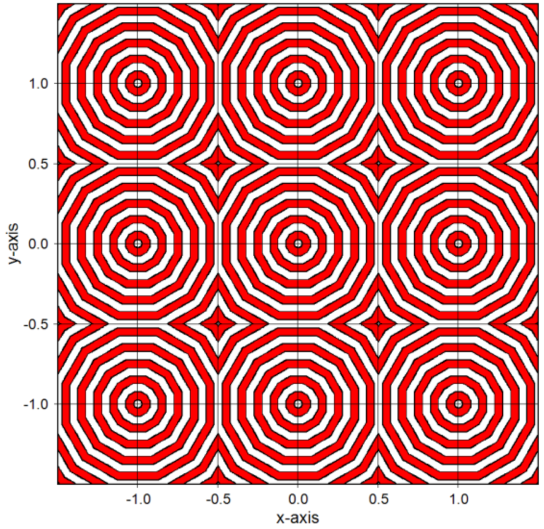
kt=11



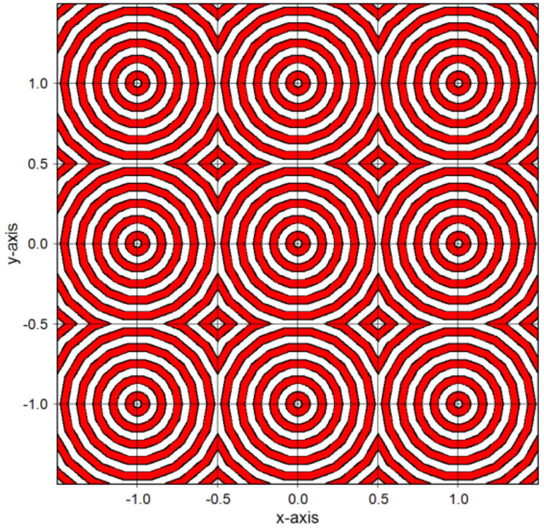
kt=12



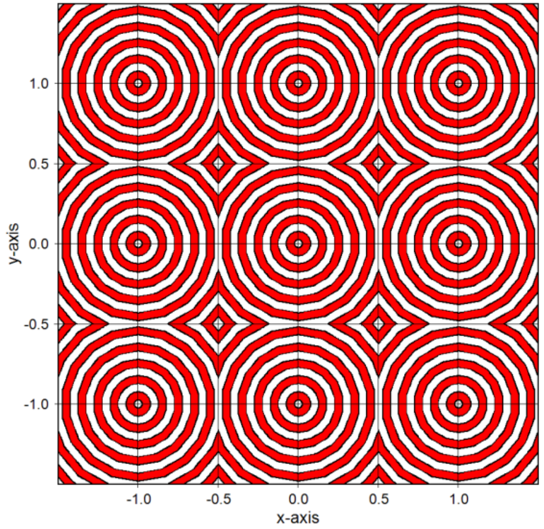
kt=13



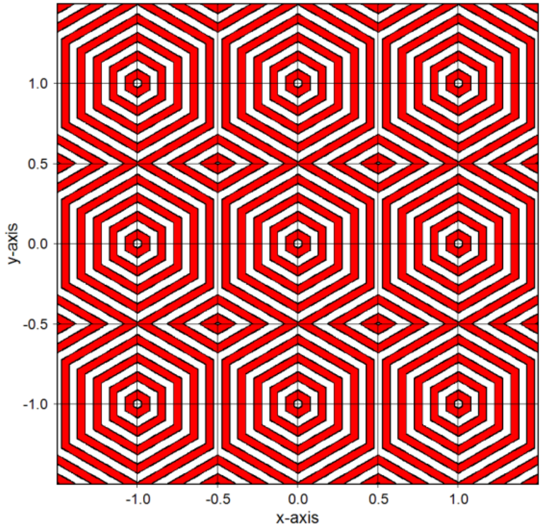
kt=14



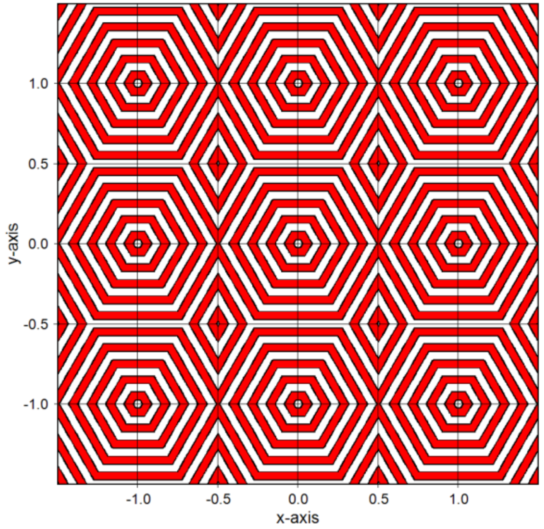
kt=15



kt=16

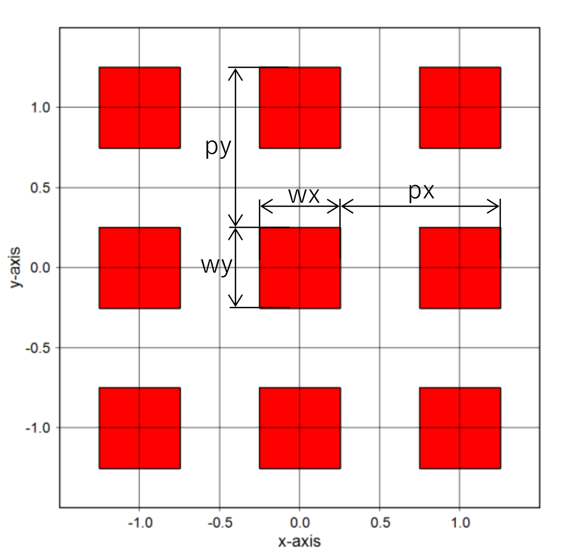


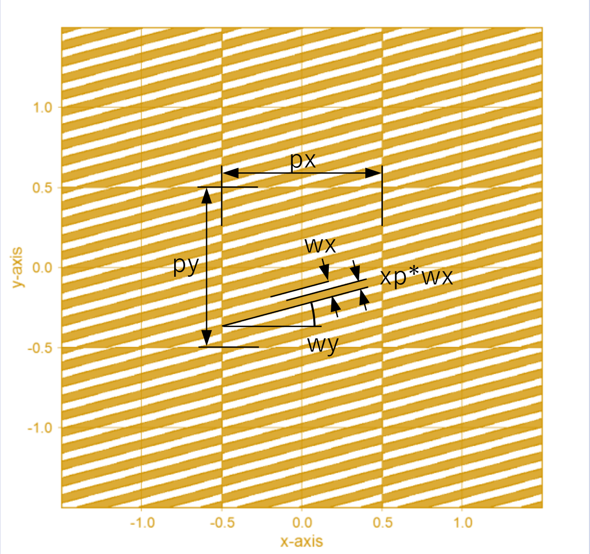
kt=17

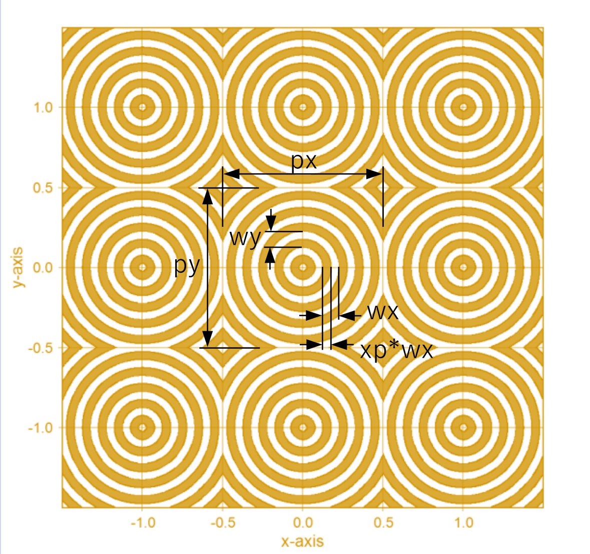


24. Relationships (4) between kt and structures for kd=0

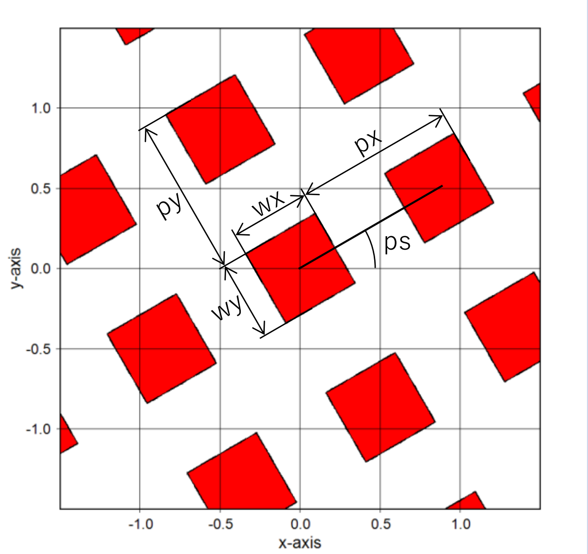
kt=1,ps=0.0	kt=10,xp=0.5	kt=11,xq=0.0

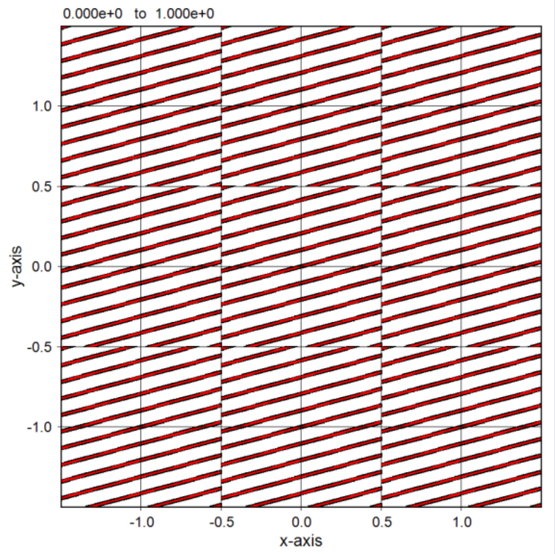


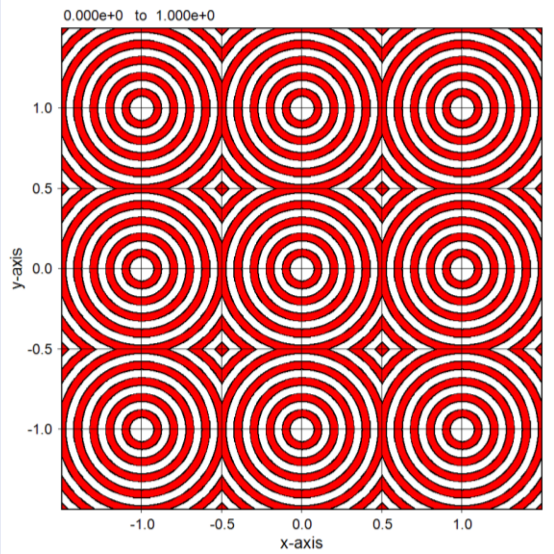




kt=1,ps=30.0	kt=10,xp=0.2	kt=11,xq=0.5







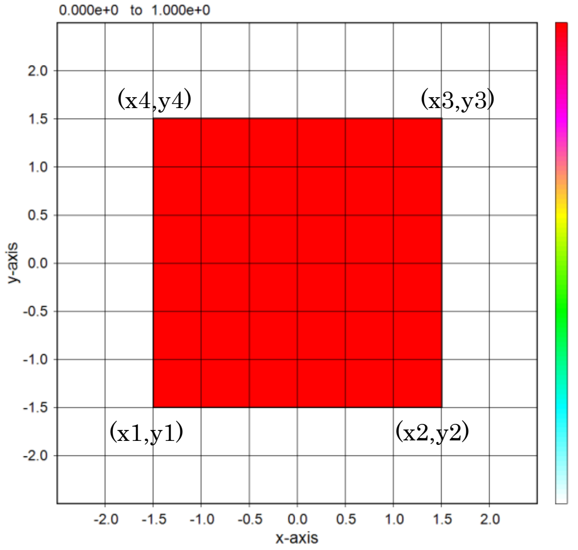
25. Reference to sub.dat for kd=1 (sub1.dat)

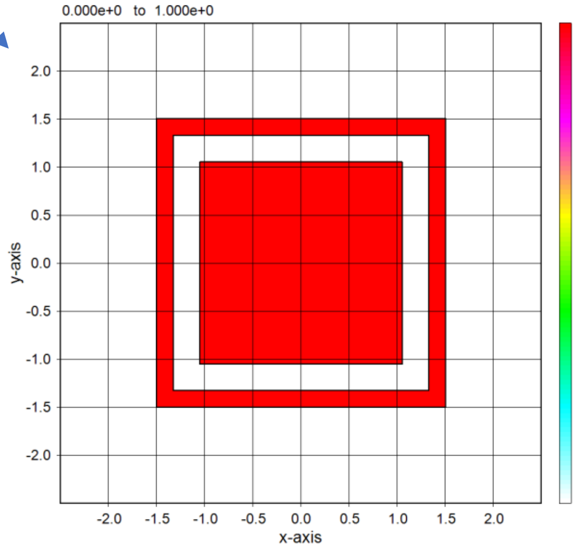
Contents of sub.dat

Digit1	5	x1 (15)	y1 (25)	x2 (35)	y2 (45)	x3 (55)	y3 (65)	x4 (75)	y4 (85)
	1	-1. 5000	-1. 5000	1. 5000	-1. 5000	1. 5000	1. 5000	-1. 5000	1. 5000
	2	-1. 0500	-1. 0500	1. 0500	-1. 0500	1. 0500	1. 0500	-1. 0500	1. 0500
		-1. 5000	-1. 5000	1. 5000	-1. 5000	1. 5000	-1. 3250	-1. 5000	-1. 3250
		1. 3250	-1. 3250	1. 5000	-1. 3250	1. 5000	1. 3250	1. 3250	1. 3250
		1. 5000	1. 3250	1. 5000	1. 5000	-1. 5000	1. 5000	-1. 5000	1. 3250
		-1. 5000	-1. 3250	-1. 3250	-1. 3250	-1. 3250	1. 3250	-1. 5000	1. 3250

Corresponding to the values kt of wsr.dat. Duplication is prohibited.

Excerpt of sub.dat





The enclosing figures of four points (in μm) of (x1,y1), (x2,y2), (x3,y3), and (x4,y4) or their aggregate figures are lined up at a pitch of px, py and a shift amount of sx, sy.

Numeric data input rules

- Input numerals must be one-byte ones (full-width spaces are not allowed, nor are tab codes).
- The right end of the input numerals for each must be aligned with 10-digits increments after first 5-digits.
- Input numbers should be separated by at least one space.

26. Method of forming a lens shape (wsr13.dat), 238s

	A	B	C	D	E
1					
2	a=radius	n=Layer No	y=a-n*dz	x=sqrt(a^2-y^2)	2x=Intercept width
3	0.75	1	0.740	0.122	0.244
4	dz=Grid interval	2	0.720	0.210	0.420
5	0.02	3	0.700	0.269	0.539
6	ht=height	4	0.680	0.316	0.633
7	0.5	5	0.660	0.356	0.712
8		6	0.640	0.391	0.782
9		7	0.620	0.422	0.844
10		8	0.600	0.450	0.900
11		9	0.580	0.475	0.951
12		10	0.560	0.499	0.998
13		11	0.540	0.520	1.041
14		12	0.520	0.540	1.081

wsems_data.xlsx

ht Structure height (μm)
a Radius for circular cross-section (μm)

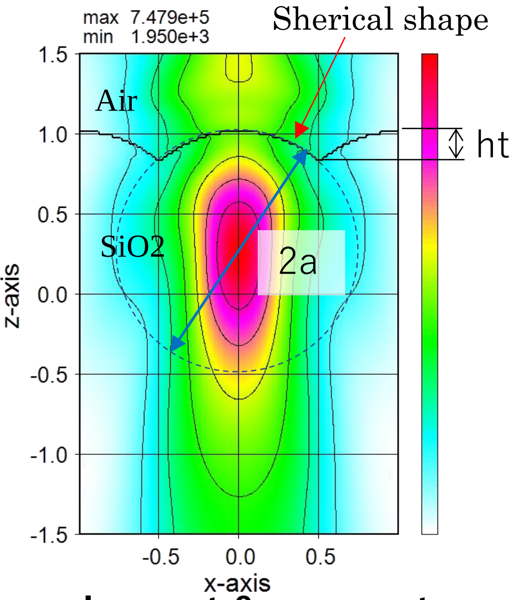
```
** wsr.dat
*        hm        trc        wb(um)     kfl(0,1)  kot       ity
         5.0       2.0        0.5        0         0         0
*        wdx(um)   wdy(um)    dxy(um)    dz(um)
         2.0       2.0        0.01       0.01
*        Lam(um)   th(deg)    fi(deg)    gm(deg)
        0.75       0.0        0.0        0.0
*        alx       aly        sx0(um)    sy0(um)
         0.5       0.5        0.0        0.0
*        stx(um)   sty(um)    csx(um)    csy(um)
         0.0       0.0        0.0        0.0
* km  *    Name    ko    an       ab     ak
   1#      Ta205   1     1.0000   0.00   0.0000
   2       -SiO2   1     1.4500   0.00   0.0000
* kr       * kd   kt    ps(deg)  px(um)  py(um)  wx(um)  wy(um)  sx(um)  sy(um)  xp
   1#        0    4     0.0      1.50    1.50    0.500   0.50    0.00    0.00    0.0
* kf   km   kr kd   kt   ps(deg)   px(um)   py(um)   wx(um)   wy(um)   sx(um)   sy(um)   xp    xq
   1    2    0  0    2    0.0       1.000    1.000    0.244    0.244    0.000    0.00     0.0   0.0
   2    2    0  0    2    0.0       1.000    1.000    0.420    0.420    0.000    0.00     0.0   0.0
   3    2    0  0    2    0.0       1.000    1.000    0.539    0.539    0.000    0.00     0.0   0.0
   4    2    0  0    2    0.0       1.000    1.000    0.633    0.633    0.000    0.00     0.0   0.0
   5    2    0  0    2    0.0       1.000    1.000    0.712    0.712    0.000    0.00     0.0   0.0
   6    2    0  0    2    0.0       1.000    1.000    0.782    0.782    0.000    0.00     0.0   0.0
   7    2    0  0    2    0.0       1.000    1.000    0.844    0.844    0.000    0.00     0.0   0.0
   8    2    0  0    2    0.0       1.000    1.000    0.900    0.900    0.000    0.00     0.0   0.0
   9    2    0  0    2    0.0       1.000    1.000    0.951    0.951    0.000    0.00     0.0   0.0
  10    2    0  0    2    0.0       1.000    1.000    0.998    0.998    0.000    0.00     0.0   0.0
  11    2    0  0    2    0.0       1.000    1.000    1.041    1.041    0.000    0.00     0.0   0.0
  12    2    0  0    2    0.0       1.000    1.000    1.081    1.081    0.000    0.00     0.0   0.0
  13    2    0  0    2    0.0       1.000    1.000    1.118    1.118    0.000    0.00     0.0   0.0
  14    2    0  0    2    0.0       1.000    1.000    1.153    1.153    0.000    0.00     0.0   0.0
  15    2    0  0    2    0.0       1.000    1.000    1.185    1.185    0.000    0.00     0.0   0.0
  16    2    0  0    2    0.0       1.000    1.000    1.215    1.215    0.000    0.00     0.0   0.0
  17    2    0  0    2    0.0       1.000    1.000    1.243    1.243    0.000    0.00     0.0   0.0
  18    2    0  0    2    0.0       1.000    1.000    1.269    1.269    0.000    0.00     0.0   0.0
  19    2    0  0    2    0.0       1.000    1.000    1.293    1.293    0.000    0.00     0.0   0.0
  20    2    0  0    2    0.0       1.000    1.000    1.316    1.316    0.000    0.00     0.0   0.0
  21    2    0  0    2    0.0       1.000    1.000    1.337    1.337    0.000    0.00     0.0   0.0
  22    2    0  0    2    0.0       1.000    1.000    1.357    1.357    0.000    0.00     0.0   0.0
  23    2    0  0    2    0.0       1.000    1.000    1.375    1.375    0.000    0.00     0.0   0.0
  24    2    0  0    2    0.0       1.000    1.000    1.392    1.392    0.000    0.00     0.0   0.0
  25    2    0  0    2    0.0       1.000    1.000    1.407    1.407    0.000    0.00     0.0   0.0
* kb  kl  km  kp     tk     kf     *   *   *   *   *   *   *   *   *   *   *   *   *   *   *   *
   1   0   0   0   0.500   000     0
```

Continued

続き

```
   2   0   0   0   0.020   001   0
   3   0   0   0   0.020   002   0
   4   0   0   0   0.020   003   0
   5   0   0   0   0.020   004   0
   6   0   0   0   0.020   005   0
   7   0   0   0   0.020   006   0
   8   0   0   0   0.020   007   0
   9   0   0   0   0.020   008   0
  10   0   0   0   0.020   009   0
  11   0   0   0   0.020   010   0
  12   0   0   0   0.020   011   0
  13   0   0   0   0.020   012   0
  14   0   0   0   0.020   013   0
  15   0   0   0   0.020   014   0
  16   0   0   0   0.020   015   0
  17   0   0   0   0.020   016   0
  18   0   0   0   0.020   017   0
  19   0   0   0   0.020   018   0
  20   0   0   0   0.020   019   0
  21   0   0   0   0.020   020   0
  22   0   0   0   0.020   021   0
  23   0   0   0   0.020   022   0
  24   0   0   0   0.020   023   0
  25   0   0   0   0.020   024   0
  26   0   0   0   0.020   025   0
  27   0   2   0   2.000   000   0
```

Rewritten　As it is　Rewritten　As it is　Rewritten



i_xz.out & m_xz.out

27. Method of converting AFM data by afm.exe (afm01.dat)

nx x-axis measurement point
ny y-axis measurement point
dx x-axis measurement increment (μm)
dy y-axis measurement increment (μm)
amp z-axis measurement amplification ratio
theta Azimuth angle of the plane normal with the z-axis (deg)
phi Angular angle of the plane normal around the z-axis (deg)
psi Rotation angle of the measured image around the plane normal (deg)

AFM measurement data of nx ·ny (for x and y-axis) points, each value in μm, displayed in 10 digits

Input file afm.dat

** AFM data

nx	ny	dx(um)	dy(um)	amp	theta(deg)	phi(deg)	psi(deg)
15	15	0.07	0.07	1.000	0.000	0.0000	0.0000

0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.007605	0.011817	0.007605	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.032162	0.064350	0.086619	0.094445	0.086619	0.064350	0.032162	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.007605	0.057395	0.110630	0.153556	0.180427	0.189501	0.180427	0.153556	0.110630	0.057395	0.007605	0.000000	0.000000
0.000000	0.000000	0.057395	0.127439	0.189501	0.235001	0.261937	0.270777	0.261937	0.235001	0.189501	0.127439	0.057395	0.000000	0.000000
0.000000	0.032162	0.110630	0.189501	0.253019	0.296660	0.321334	0.329225	0.321334	0.296660	0.253019	0.189501	0.110630	0.032162	0.000000
0.000000	0.064350	0.153556	0.235001	0.296660	0.336921	0.358735	0.365534	0.358735	0.336921	0.296660	0.235001	0.153556	0.064350	0.000000
0.007605	0.086619	0.180427	0.261937	0.321334	0.358735	0.378339	0.384319	0.378339	0.358735	0.321334	0.261937	0.180427	0.086619	0.007605
0.011817	0.094445	0.189501	0.270777	0.329225	0.365534	0.384319	0.390000	0.384319	0.365534	0.329225	0.270777	0.189501	0.094445	0.011817
0.007605	0.086619	0.180427	0.261937	0.321334	0.358735	0.378339	0.384319	0.378339	0.358735	0.321334	0.261937	0.180427	0.086619	0.007605
0.000000	0.064350	0.153556	0.235001	0.296660	0.336921	0.358735	0.365534	0.358735	0.336921	0.296660	0.235001	0.153556	0.064350	0.000000
0.000000	0.032162	0.110630	0.189501	0.253019	0.296660	0.321334	0.329225	0.321334	0.296660	0.253019	0.189501	0.110630	0.032162	0.000000
0.000000	0.000000	0.057395	0.127439	0.189501	0.235001	0.261937	0.270777	0.261937	0.235001	0.189501	0.127439	0.057395	0.000000	0.000000
0.000000	0.000000	0.007605	0.057395	0.110630	0.153556	0.180427	0.189501	0.180427	0.153556	0.110630	0.057395	0.007605	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.032162	0.064350	0.086619	0.094445	0.086619	0.064350	0.032162	0.000000	0.000000	0.000000	0.000000
0.000000	0.000000	0.000000	0.000000	0.000000	0.000000	0.007605	0.011817	0.007605	0.000000	0.000000	0.000000	0.000000	0.000000	0.000000

Execution file afm.exe

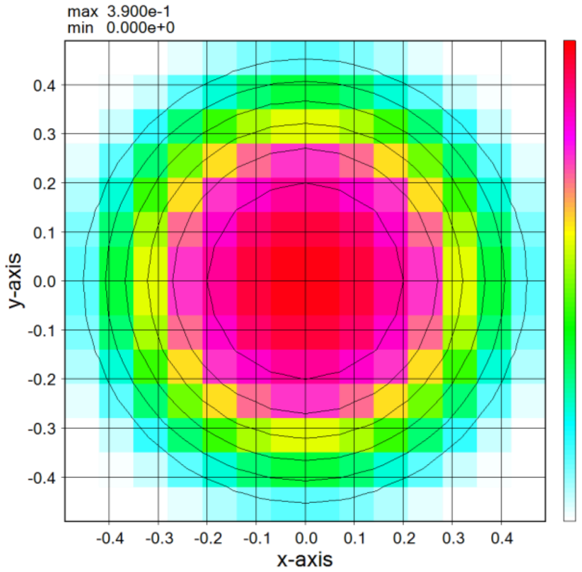
Click to generate (overwrite) the output file in a folder

Output file

afm.out For being pasted into sub.dat.

afm_xy.out AFM data before and after correction which Wscnt visualizes as 1st and 2nd picture.

In case of theta=phi=psi=0, AFM data is the same before and after correction and one is selected.



afm_xy.out 2nd picture visualized by Wscnt

28. Pasting converted data of AFM (wsr14.dat), 32s

```
** wsr.dat
*       hm        trc        wb(um)    kfl(0,1)   kot      ity
       5.0        2.0        0.0         0        0         0
*     wdx(um)   wdy(um)    dxy(um)     dz(um)
       2.0        2.0       0.01       0.01
*     Lam(um)    th(deg)    fi(deg)    gm(deg)
      0.75        0.0        0.0        0.0
*      alx        aly       sx0(um)    sy0(um)
       0.5        0.5        0.0        0.0
*     stx(um)    sty(um)    csx(um)    csy(um)
       0.0        0.0        0.0        0.0
* km    *    Name   ko      an         ab       ak
   1#       Ta205    1    1.0000      0.00    0.0000
   2        -Si02    1    1.4500      0.00    0.0000
* kr        * kd   kt    ps(deg)    px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)    xp
   1#          0    4     0.0        1.50      1.50      0.500     0.50      0.00      0.00      0.0
* kf  km   kr kd   kt    ps(deg)    px(um)    py(um)    wx(um)    wy(um)    sx(um)    sy(um)    xp     xq
   1   2    0  1   11     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
   2   2    0  1   12     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
   3   2    0  1   13     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
   4   2    0  1   14     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
   5   2    0  1   15     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
   6   2    0  1   16     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
   7   2    0  1   17     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
   8   2    0  1   18     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
   9   2    0  1   19     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  10   2    0  1   20     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  11   2    0  1   21     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  12   2    0  1   22     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  13   2    0  1   23     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  14   2    0  1   24     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  15   2    0  1   25     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  16   2    0  1   26     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  17   2    0  1   27     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  18   2    0  1   28     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
  19   2    0  1   29     0.0        1.00      1.00      0.00      0.00      0.000     0.00      0.0    0.0
* kb  kl  km  kp      tk     kf    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
   1   0   0   0    0.500    0    0
```

Continued

```
 2   0   0   0.0200    1   0
 3   0   0   0.0200    2   0
 4   0   0   0.0200    3   0
 5   0   0   0.0200    4   0
 6   0   0   0.0200    5   0
 7   0   0   0.0200    6   0
 8   0   0   0.0200    7   0
 9   0   0   0.0200    8   0
10   0   0   0.0200    9   0
11   0   0   0.0200   10   0
12   0   0   0.0200   11   0
13   0   0   0.0200   12   0
14   0   0   0.0200   13   0
15   0   0   0.0200   14   0
16   0   0   0.0200   15   0
17   0   0   0.0200   16   0
18   0   0   0.0200   17   0
19   0   0   0.0200   18   0
20   0   0   0.0200   19   0
21   2   0   2.000     0   0
```

Input file

afm.dat

paste

sub.dat

afm.out

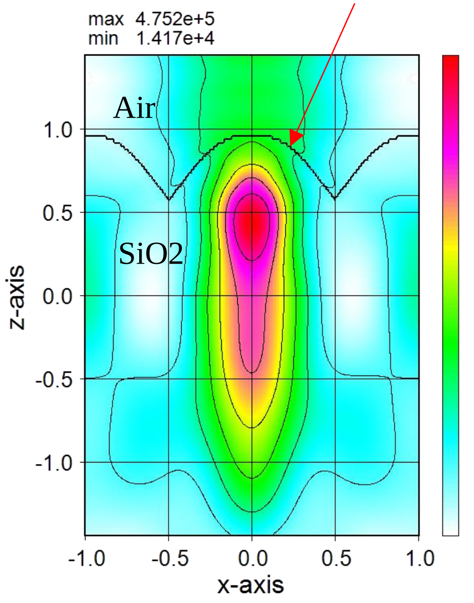
Output file

Rewritten

As it is

Rewritten

Measurement shape of AFM expressed by sub.dat

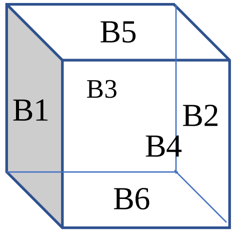


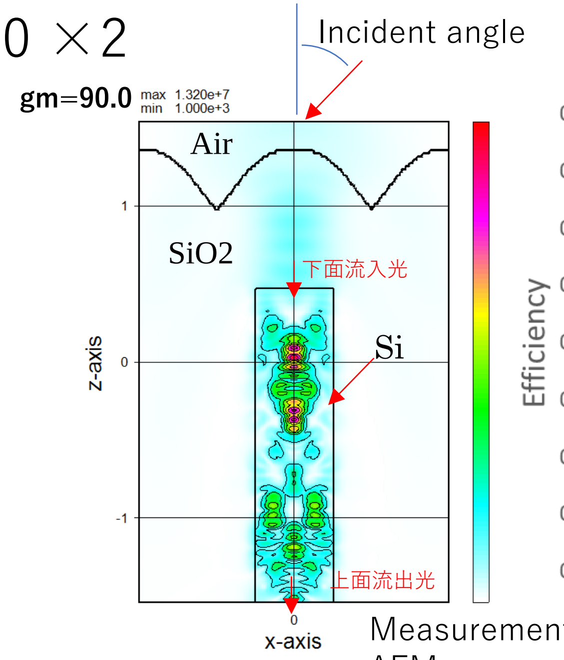
i_xz.out & m_xz.out

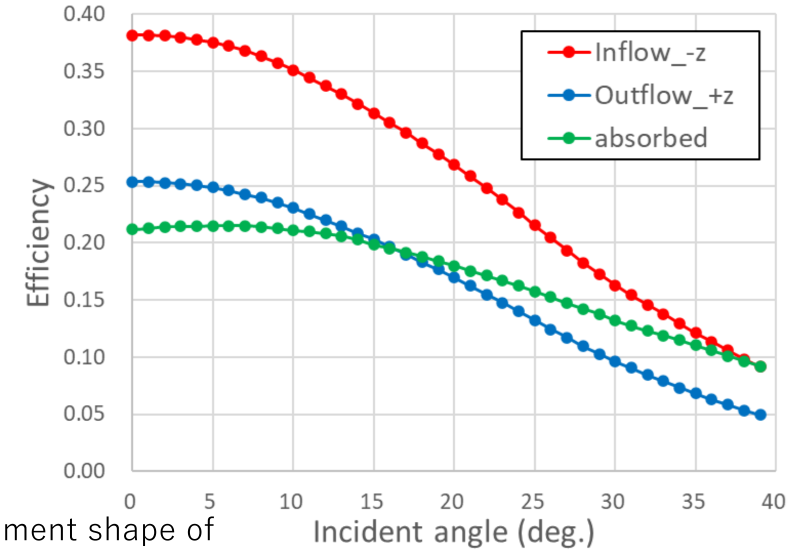
29. Calculation example (wsr15.dat), 213s×40 ×2

```
** wsr.dat
*       hm          trc          wb(um)    kfl(0,1)  kot         ity
        5.0         2.0         0.5          0         0          0
*       wdx(um)     wdy(um)     dxy(um)    dz(um)
        2.0         2.0        0.01        0.01
*       Lam(um)     th(deg)     fi(deg)    gm(deg)
       0.75         0.0         0.0        0.0
*       alx         aly         sx0(um)    sy0(um)
        0.3         0.3         0.0        0.0
*       stx(um)     sty(um)     csx(um)    csy(um)
        0.0         0.0         0.0        0.0
* km    *     Name  ko          an         ab        ak
   1            Si   1      1.0000       0.00    0.0000
   2          -SiO2  1      1.4500       0.00    0.0000
* kr           * kd   kt     ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)     xp
   1#             0    4       0.0       1.50       1.50      0.500       0.50       0.00       0.00      0.0
* kf    km    kr kd   kt     ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)     xp         xq
   1     2     0  1   11       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
   2     2     0  1   12       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
   3     2     0  1   13       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
   4     2     0  1   14       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
   5     2     0  1   15       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
   6     2     0  1   16       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
   7     2     0  1   17       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
   8     2     0  1   18       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
   9     2     0  1   19       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  10     2     0  1   20       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  11     2     0  1   21       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  12     2     0  1   22       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  13     2     0  1   23       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  14     2     0  1   24       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  15     2     0  1   25       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  16     2     0  1   26       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  17     2     0  1   27       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  18     2     0  1   28       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  19     2     0  1   29       0.0       1.00       1.00       0.00       0.00      0.000       0.00      0.0        0.0
  20     1     0  0    1       0.0        0.0        0.0       0.50       0.50      0.000       0.00      0.0        0.0
* kb    kl    km    kp        tk     kf      *     *     *     *     *     *     *     *     *     *     *     *     *     *     *
   1     0     0     0     0.200      0      0
   2     0     0     0    0.0200      1      0
   3     0     0     0    0.0200      2      0
   4     0     0     0    0.0200      3      0
   5     0     0     0    0.0200      4      0
   6     0     0     0    0.0200      5      0
   7     0     0     0    0.0200      6      0
   8     0     0     0    0.0200      7      0
   9     0     0     0    0.0200      8      0
  10     0     0     0    0.0200      9      0
  11     0     0     0    0.0200     10      0
  12     0     0     0    0.0200     11      0
  13     0     0     0    0.0200     12      0
  14     0     0     0    0.0200     13      0
  15     0     0     0    0.0200     14      0
  16     0     0     0    0.0200     15      0
  17     0     0     0    0.0200     16      0
  18     0     0     0    0.0200     17      0
  19     0     0     0    0.0200     18      0
  20     0     0     0    0.0200     19      0
  21     0     2     0     0.500      0      0
  22     0     2     0     2.000     20      0
```

When up/down is set to a reversal mode in Wscnt, “up” is correspond to -z side and “down” is to +z side.

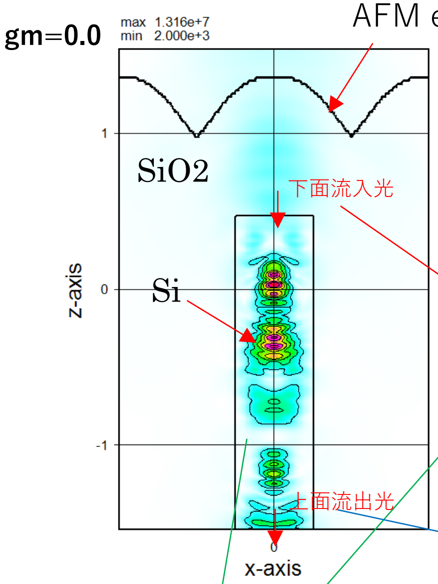


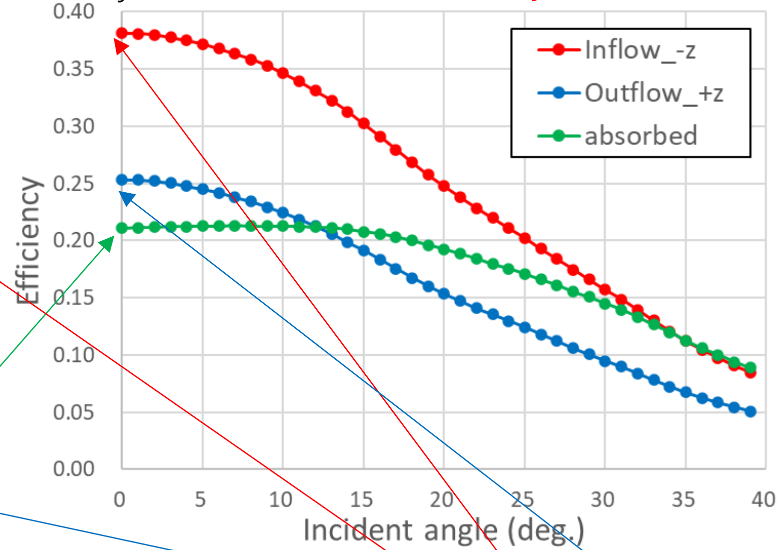




Measurement shape of AFM expressed by sub.dat

lower accuracy sue to small hm





i_xz.out & m_xz.out

Results of wsr1.out (Detected light amount)

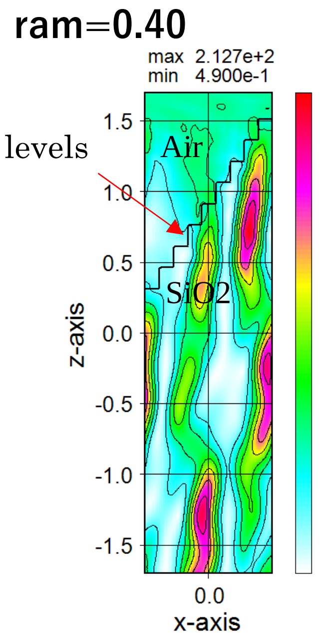
Transmitted	Reflected	Absorbed	Total	Absorbed_M01	Inflow_M01_-x	Inflow_M01_+x	Inflow_M01_-y	Inflow_M01_+y	Inflow_M01_-z	Inflow_M01_+z
4.9555E-01	2.8341E-02	4.7611E-01	1.0000E+00	2.1114E-01	1.8228E-02	1.8035E-02	2.4718E-02	2.2110E-02	3.8122E-01	-2.5317E-01

wsr1.out

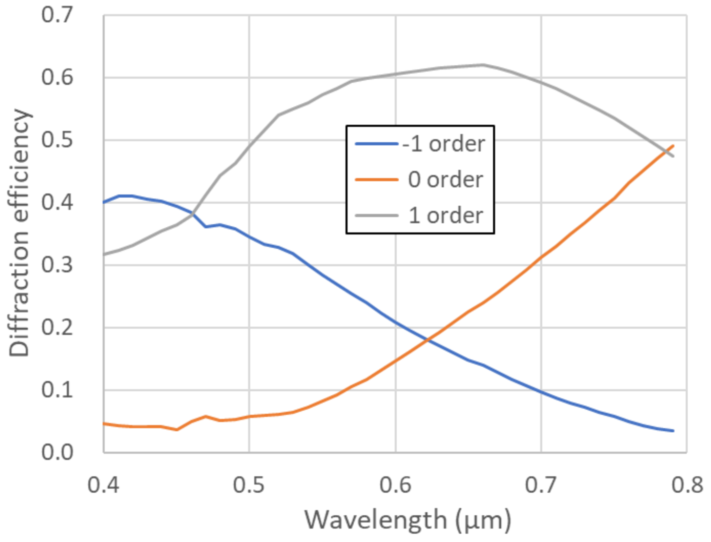
30. Calculation example (wsr16.dat), 1.1s×40

```
** wsr.dat
*        hm        trc         wb(um)    kfl(0,1)  kot        ity
         5.0       2.0         0.0         0         0          0
*        wdx(um)   wdy(um)     dxy(um)    dz(um)
         0.9       0.0        0.01       0.01
*        Lam(um)    th(deg)    fi(deg)    gm(deg)
         0.4       0.0         0.0        0.0
*        alx       aly         sx0(um)    sy0(um)
         1.0       1.0         0.0        0.0
*        stx(um)   sty(um)     csx(um)    csy(um)
         0.0       0.0         0.0        0.0
* km   *    Name  ko         an          ab         ak
   1       -SiO2   1     1.4500        0.00     0.0000
* kr          * kd    kt       ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)     xp
   1#            0     4       0.0        1.50       1.50      0.500       0.50       0.00       0.00       0.0
* kf    km    kr kd    kt       ps(deg)    px(um)     py(um)     wx(um)     wy(um)     sx(um)     sy(um)     xp         xq
   1     1     0  0     1       0.0        0.90       1.00       0.10       1.00      0.400       0.00       0.0        0.0
   2     1     0  0     1       0.0        0.90       1.00       0.20       1.00      0.350       0.00       0.0        0.0
   3     1     0  0     1       0.0        0.90       1.00       0.30       1.00      0.300       0.00       0.0        0.0
   4     1     0  0     1       0.0        0.90       1.00       0.40       1.00      0.250       0.00       0.0        0.0
   5     1     0  0     1       0.0        0.90       1.00       0.50       1.00      0.200       0.00       0.0        0.0
   6     1     0  0     1       0.0        0.90       1.00       0.60       1.00      0.150       0.00       0.0        0.0
   7     1     0  0     1       0.0        0.90       1.00       0.70       1.00      0.100       0.00       0.0        0.0
   8     1     0  0     1       0.0        0.90       1.00       0.80       1.00      0.050       0.00       0.0        0.0
* kb  kl  km  kp       tk    kf    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *    *
   1   0   0   0    0.200     0    0
   2   0   0   0  0.15000     1    0
   3   0   0   0  0.15000     2    0
   4   0   0   0  0.15000     3    0
   5   0   0   0  0.15000     4    0
   6   0   0   0  0.15000     5    0
   7   0   0   0  0.15000     6    0
   8   0   0   0  0.15000     7    0
   9   0   0   0  0.15000     8    0
  10   0   1   0    2.000     0    0
```

Blazed grating with 8 levels



i_xz.out & m_xz.out



Results of wsr2.out (Diffraction efficiency)

31. Notes

1. Internally defined materials (SiO_2, Ag, Al, Au, Be, Cr, Cu, Ni, Pd, Pt, Ti, W) are prefixed with -, like -Ag. This is done to distinguish from externally definitions.
2. When defining the same material in nk.dat as the internal one, change the material name from that of the internal one.
3. If an execution error occurs, please check the following items.
   a. Do input numbers contain half-width ones?
   b. Is the right edge of an input number aligned with the right edge of the variable label (or the * mark) above?
   c. Is the type of input digits (integer type or real number type) correct? An integer type is without a decimal point, and a real number type with a decimal point.
   d. Are there any numbers not specified in km, kb, or kf specification fields?