2D binary grating

We consider 2D binary grating from paper: Song *Peng* and G. Michael *Morris*. *JOSA A*, Vol. 12, Issue 5, pp. 1087-1096 (*1995)*. Parameters of the grating and calculation are folowing: wavelength λ=1 μm, thickness d=1 μm, periods $\Lambda_x=\Lambda_y$=1.2 μm, incident angle θ=0º, refractive index of the incident region n_1=1, refractive index of the transmission region n_3=1.5, conical angle φ=0°, polarization angle ψ=90° and 50% duty cycle (n=1.5) along the *x* and the *y* axis.

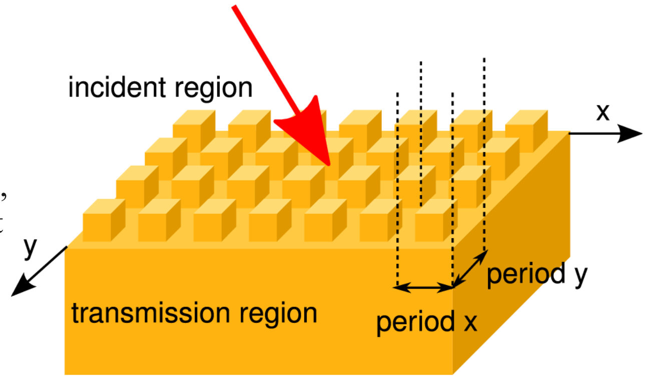


Figure 1: Definition of a crossed grating.

Grating is defined in the file peng_simple_dielectric_grating.m (directory /structures)

```
number_of_layers=1;

l=1; % layer 1
thickness(l)=1;

coordinate_x_1=1.2.*[0,0.25,0.75,1];
coordinate_y_1=1.2.*[0,0.25,0.75,1];

r_index_1=[1, 1, 1;
    1, 1.5, 1;
    1, 1, 1];
```

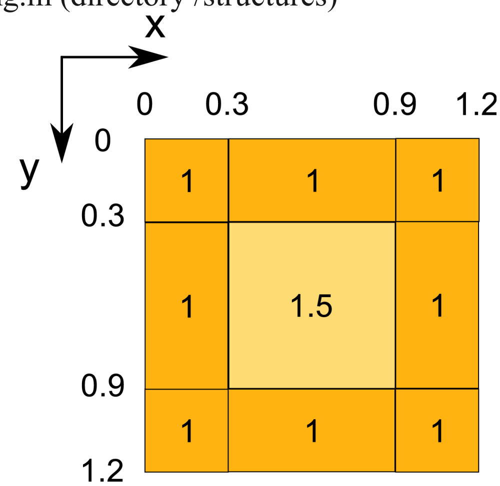


Figure 2: Discretization of a grating.

Variable *coordinate_x_1* defines x-axis coordinate of the grating (see Fig. 2), variable *coordinate_y_1* defines y-axis coordinate of the grating, variable *r_index_1* defines refractive index of the own grating. Rows of the matrix *r_index_1* represent refractive indicies in the x-axis direction, columns of the matrix *r_index_1* represent refractive indicies in the y-axis direction.

Next, we set others parameters in the main.m file:

```
N_X=5; % N_X=20 takes approx. 8 GB of memory

n_1=1.0; % superstrate
n_3=1.5; % substrate

lambda=1;
theta0=0; % incident angle [degree], if theta=0 -> theta0+1E-10
phi0=0; % conical angle [degree]
psi0=90;  % polarization angle [degree], 0-TM polarization, 90-TE polarization

grating=0;
switch grating
    case 0
```

```
…
open_grating_file='peng_simple_dielectric_grating.m';
```

```
measurement=0;

diffraction_efficiency_order=[0,0];
```

We obtain this result:

```
order  [ 0.00,  0.00] R_0=0.0027488206 T_0=0.2321819422 sumR=0.0172254040
sumT=0.9827745960 R_90=0.0027488206 T_90=0.2321819422 sumR=0.0172254040
sumT=0.9827745960 R_psi=0.0027488206 T_psi=0.2321819422 sumR=0.0172254040
sumT=0.9827745960

time of calculation = 2.470000e+00 s
```

This result is only for order [0,0], the first set of results are for ψ=0° (TM polarization), the second set of results are for ψ=90° (TE polarization), and the third set of results are for certain angle ψ which is defined in the file main.m. Another order (e.g. [-1,0]) can be displayed using variable another_diffraction_efficiency_order.

```
>> another_diffraction_efficiency_order([-1,0])

order  [-1.00,  0.00] R_0=0.0057446268 T_0=0.1550288046 sumR=0.0172254040
sumT=0.9827745960 R_90=0.0014936648 T_90=0.1690707065 sumR=0.0172254040
sumT=0.9827745960 R_psi=0.0014936648 T_psi=0.1690707065 sumR=0.0172254040
sumT=0.9827745960
```

Complete solution for all real diffraction orders can be obtained by using the commands `total_D_R_0`, `total_D_R_90`, `total_D_R`, `total_D_T_0`, `total_D_T_90`, `total_D_T`. For example, complete solution of all transmitted orders (TE polarization) is following

```
>>  total_D_T_90

total_D_T_90 =

  -1.000000000000000  -1.000000000000000   0.025598407906076
  -1.000000000000000                   0   0.155028804579578
  -1.000000000000000   1.000000000000000   0.025598407906077
                   0  -1.000000000000000   0.169070706525881
                   0                   0   0.232181942160683
                   0   1.000000000000000   0.169070706525886
   1.000000000000000  -1.000000000000000   0.025598407906021
   1.000000000000000                   0   0.155028804578851
   1.000000000000000   1.000000000000000   0.025598407906021
```

more layers: eg. Grating (thickness 0.5)+Grating (thickness 0.5)+uniform layer

```
number_of_layers=3;

l=1; % layer 1
thickness(l)=0.5;

coordinate_x_1=1.2.*[0,0.25,0.75,1];
coordinate_y_1=1.2.*[0,0.25,0.75,1];

r_index_1=[1, 1, 1;
    1, 1.5, 1;
```

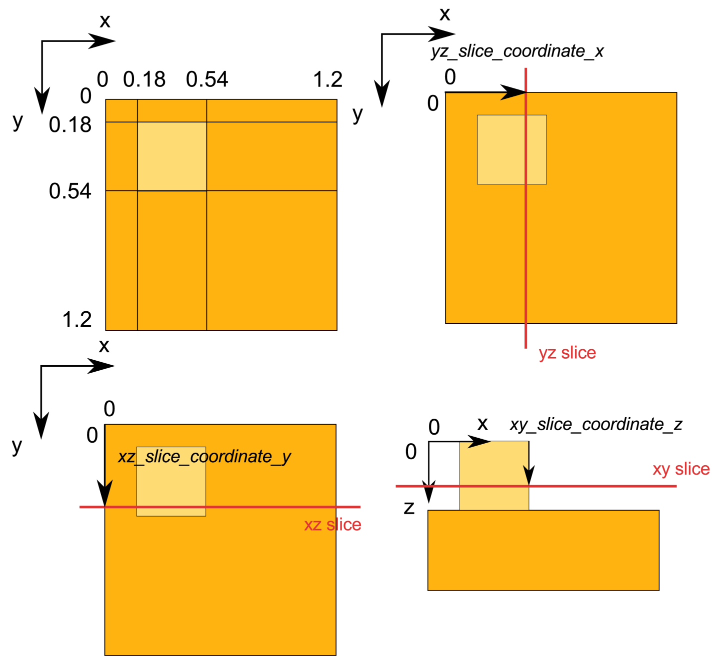
```
    1, 1, 1];


l=2; % layer 2
thickness(l)=0.5;

coordinate_x_2=1.2.*[0,0.25,0.75,1];
coordinate_y_2=1.2.*[0,0.25,0.75,1];

r_index_2=[1, 1, 1;
    1, 1.5, 1;
    1, 1, 1];

l=3; % layer 3
thickness(l)=0.5;

coordinate_x_3=1.2.*[0,1];
coordinate_y_3=1.2.*[0,1];

r_index_3=[1.5];
```

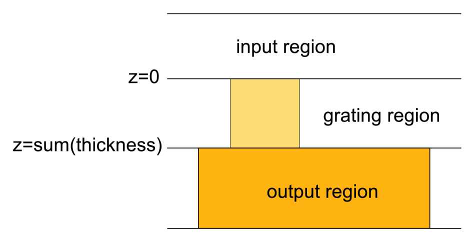
Field calculation

Add some text

some notes on field calculation:

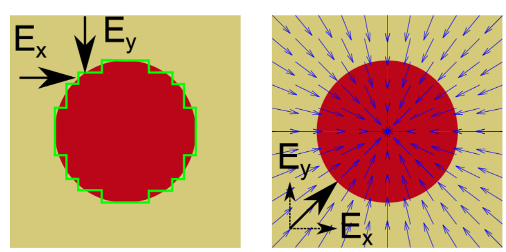
- example: main_binary_grating_em_field.m
- calculate_field=1 → it enables field calculation
- run the main_binary_grating_em_field.m file and open (directory /em_field) xy_slice.m or xz_slice.m or yz_slice.m → change variables in slice *.m files and run these files (all grating variables are in memory)
- field components: E_x, E_y, E_z, H_x, H_y, H_z
- field components can be calculated in input region, grating region, and output region
- field calculation is done for polarization angle psi0

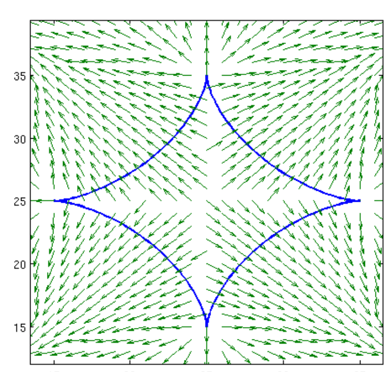




Normal vector method

Todo





T. Schuster, J. Ruoff, N. Kerwien, S. Rafler, W. Osten, "Normal vector method for convergence improvement using the RCWA for crossed gratings," J. Opt. Soc. Am. A **24**, 2880-2890 (2007)

R. Antoš, "Fourier factorization with complex polarization bases in modeling optics of discontinuous bi-periodic structures," Opt. Express **17**, p. 7269, 2009

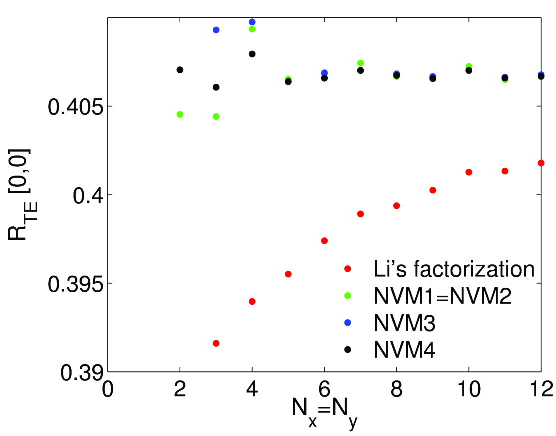
P. Götz, T. Schuster, K. Frenner, S. Rafler, and W. Osten, "Normal vector method for the RCWA with automated vector field generation," Opt. Express **16**, 17295-17301 (2008).

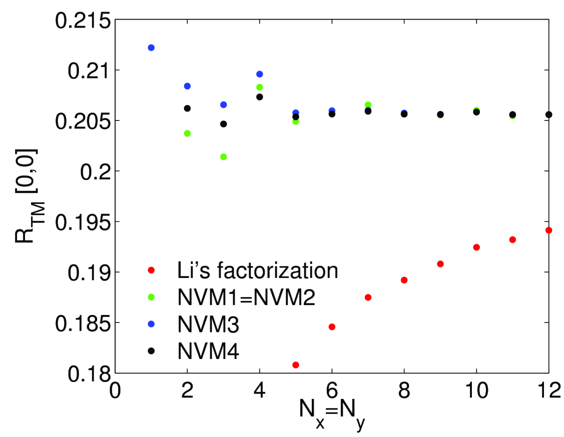
S. Rafler, P. Goetz, M. Petschow, T. Schuster, K. Frenner, W. Osten, "Investigation of methods to set up the normal vector field for the differential method," Proc. SPIE, Vol. 6995, 2008

This example is taken from paper: R. Antos, M. Veis, S. Visnovsky, "Complex Fourier factorization method applied in modeling optical metamaterials based on 2D periodic nanostructures," Proc. SPIE, Vol. 7353 73531C-2, 2009. We suppose cylindrical holes of the diameter 2R = 200 nm, depth d = 100 nm, and square periodicity Λ = 300 nm. We assume an incident plane wave with the wavelength λ = 500 nm, the angle of incidence θ=60° , and the conical angle φ=0°. As material parameters at our spectral point we use the values of permittivity, ε_a = 1 for vacuum inside holes (+ incident region) and ε_b = −2. 865−3. 211i for outside holes (+ transmission region).

Setup of the structure is saved in the test_antos_grating.m file. A similar input file is deeply described in the next section. This example is run from the main_nvm.m file. In the case of cylindrical holes/rods, program RCWA-2D offers three independent setups of the normal vector fields – switch `factorization_method`.

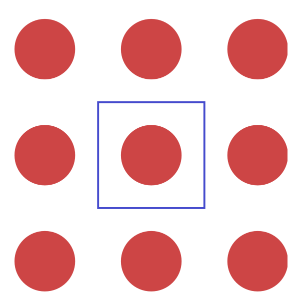
1) radial normal vector field
2) complex radial normal vector field (same as the case 1)
3) complex normal vector field based on complex polarization bases (Model C)
4) complex normal vector field based on complex polarization bases (Model C')





Circular holes/rods – rectangular grid

Let us assume simple case of the grating (Λ_x=Λ_y=1.0 μm) consists of circular air holes (radius r=0.25 μm, thickness t=1 μm) in the dielectric medium



(n=1.5). Program RCWA-2D provides two ways, how to calculate such a grating. Firstly, this grating with circular hole/rod can be discretized, then we can immediately use previous algorithm based on

Lifeng Li, "New formulation of the Fourier modal method for crossed surface-relief gratings," J. Opt. Soc. Am. A **14**, 2758-2767 (1997),

or fourier coefficients of such a grating can be calculated using Bessel functions and then we have to apply an algorithm based on

Philippe Lalanne, "Improved formulation of the coupled-wave method for two-dimensional gratings," J. Opt. Soc. Am. A **14**, 1592-1598 (1997).

We first discuss the first posibility, the setup of the grating is the same as in the previous case of 2D binary grating. You have to only load rectangular_grating.m file.

```
open_grating_file='rectangular_grating.m';
```

Strucure of the rectangular_grating.m file:

```
number_of_layers=1; % this parameter defines number of layers
Lambda_x=1; %  [um]
Lambda_y=Lambda_x; %  [um]

resolution_dx=128; % discretization step [um]

r_cylinder=0.25; % radius of the cylinder [um]
t_cylinder=1; % thickness of the cylinder [um]

n_cylinder=1; % refractive index of the cylinder
n_layer=1.5; % refractive index of the surrounding layer

show_grating_mesh=2; % 1-yes, 2-no

%-----------------------------------------------------------
% generation of refractive index mesh
addpath('structures_scripts')
[p_x,p_y,mesh_n_mat]=rectangular_grid(Lambda_x,Lambda_y,resolution_dx,r_cylinder,n_cylinder,n_layer,show_grating_mesh);
%-----------------------------------------------------------

% definition of layer number 1
l=1;

nvm_method(l)=1; % 1=normal vector method is on (only in this layer)
factorization_method=1; % 1-radial, 2-complex radial, 3-
[N_x_input,N_y_input]=rectangular_grid_nvm(Lambda_x,Lambda_y,resolution_dx,factorization_method,r_cylinder);


thickness(l)=t_cylinder; % thickness of the layer

coordinate_x_1=p_x;
coordinate_y_1=p_y;
```

```
r_index_1=mesh_n_mat; % matrix of the refrative index grid
```

```
if theta=0 set-> theta0=1e-6; % incident angle [degree], if theta=0
```

If you want to check the discretization of your grating, then set `show_grating_mesh=1;` and run this file. You obtain a picture like Fig. 3. Sometimes you need to add a substrate layer, e.g. with refractive index 1.5 and thickness 2 μm. Firstly, set the parameter

```
number_of_layers=2;
```

and then add something like this:

```
% definition of layer number 2
l=2;

thickness(l)=2; % thickness of the layer

coordinate_x_2=[0,Lambda_x];
coordinate_y_2=[0,Lambda_y];
```

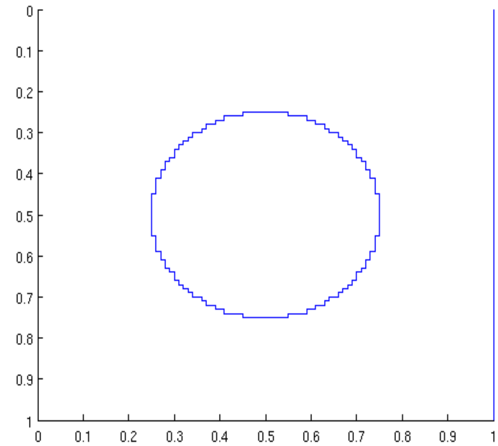


Figure 3: Discretization of a circular shape

```
r_index_2=[1.5]; % matrix of the refrative index grid
```

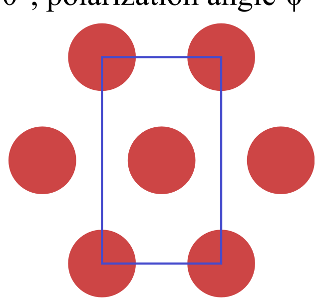
Now, we discuss the the second posibility based on Bessel function and Lalanne's algorithm. Set grating=0 in the file main.m and then you can change the parameters according to your needs, in our case

```
case 1 % eliptic cylinder, rectangular grating
        number_of_layers=1;
        setup_dispersion;
        n_layer=1.5; % refractive index of the surrounding layer
        n_cylinder=1; % refractive index of the cylinder
        thickness=1; % [um]
        a_ellipse=0.25; % semi-axis [um]
        b_ellipse=0.25; % semi-axis [um]
```

Next, Lalanne's paper intoduces new convergence parametr α. This parameter is a real positive number in the interval [0,1]. For this symmetrical configuration, α is chosen equal to 0.5. (add more information). If we compare both algorithms, the first algoritm is faster for larger number of orders N_X and more “accurate” for metallic grating.

Circular holes/rods – hexagonal grid

Let us next consider a grating that consists of round rods arranged to have a hexagonal symmetry, as shown in Fig. 2. The grating parameters are wavelength λ=0.5 μm, thickness h=λ, periods $\Lambda_x=\Lambda_y=2\lambda$, incident angle θ=30º, refractive index of the incident region n_1=1, refractive index of the transmission region n_3=sqrt(2.56), conical angle φ=30°, polarization angle ψ=90° , and the rods have a radius of λ/2.



Structural symmetries + adaptive spatial resolution technique

We consider square coaxial apertures in a metallic film, this example is adopted from paper: Gérard Granet and Lifeng Li. J. Opt. A: Pure Appl. Opt., Vol. 12, pp. 546-549 (2006*)*. Parameters of the grating and calculation are folowing: wavelength λ=0.54 μm, thickness h=0.15 μm, periods $\Lambda_x=\Lambda_y$=0.3 μm, w_1=0.155 μm, w_2=0.105 μm, n_2=0.22-6.71i (todo n_2=0.0187-3.8069i → it does not work properly), incident angle θ=0º, refractive index of the incident region n_1=1, refractive index of the transmission region n_3=1.45.

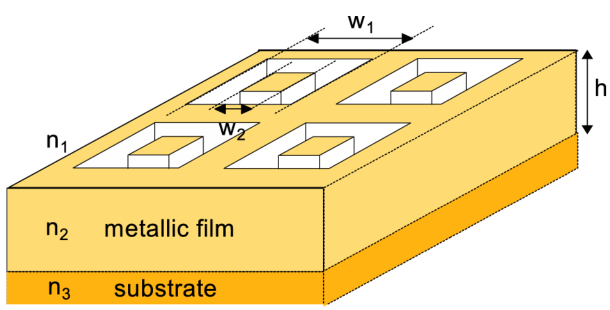


Figure 5: Definition of a structure

Let us study convergence of the zero-zero order. The structure is defined in the *coaxial_apertures_array.m* file

```
number_of_layers=1;

mu=1;
lambda=0.54;
n_1=1;
n_3=1.45;
theta0=0.0;

l=1; % layer 1
thickness(l)=0.15;

Lambda_x=0.3;
Lambda_y=Lambda_x;

w_1=0.155;
w_2=0.105;

coordinate_x_1=[0,Lambda_x/2-w_1/2,Lambda_x/2-
w_2/2,Lambda_x/2+w_2/2,Lambda_x/2+w_1/2,Lambda_x];
coordinate_y_1=coordinate_x_1;

n_ag=0.22-6.71*1i;%0.0187+3.8069*1i; % todo correct convention
```

```
r_index_1=[n_ag, n_ag, n_ag, n_ag, n_ag;
    n_ag, 1, 1, 1, n_ag;
    n_ag, 1, n_ag, 1, n_ag;
    n_ag, 1, 1, 1, n_ag;
    n_ag, n_ag, n_ag, n_ag, n_ag];
```

The convergence of the order [0,0] is shown in Fig. 6 (blue line).

Now, we will use another code:
http://sourceforge.net/projects/rcwa-2d/files/rcwa_2d_asr_sym/
This RCWA version is based on the use of the adaptive spatial resolution technique. The adaptive spatial resolution (ASR) techique is widely used in the RCWA method to reduce the Gibbs phenomenon (overshooting) around the discontinuities of the permittivity thereby to improve the convergence of the Fourier series, finaly improving the accuracy of the computation result.

In certain cases, specifically when a strucure to be modeled possesses proper symmetries, both issues of memory requirements and computational time can be reduced by taking advantage of these symmetries. In our case of the RCWA method, a strucure to be modeled must possess two separate types of symmetries concurrently, structural symmetry and input wave symmetry, in order to take advantage of either.

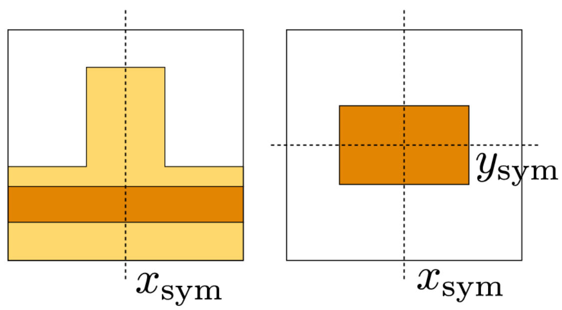


Figure 5: Schematic view of structural symmetries applied: x-axis mirror-reflection symmetry, application of both symmetries

In a 2D periodic medium, there is a possibility of the occurrence of two types of one-dimensional transverse symmetries. When the material property distribution has a mirror symmetry along the x-axis of the computational window, the system is said to possess x-axis symmetry (or σ_x symmetry), and similarly when mirror symmetry is present about the y-axis, the system is said to possess y-axis symmetry (or σ_y symmetry). For a system possessing material symmetry along the x- and y-axis simultaneously, the presence of a field that is polarized along either the x- or y-axis creates also the possibility of an even further reduction in the size of the coupled wave equation eigenmode problem. The system is said to possess (x + y)-axis symmetry (or C2v symmetry).

ASR setup: there is a stretching coefficient ASR_G in the interval (0, 1). It's choice can be used to tune and optimize the ASR performance. questions about choosing the proper value of parameter ASR_G Unfortunately no scheme exists so far to predict the optimum choice of parameters ASR_G for the ASR transformation, according to our experience, the parametr ASR_G should be close to zero (e.g. 0.05).

Next, we set others parameters in the main.m file:

```
%---------------------------------------------------
N_X=10; % memory 8 GB:  symmetry=2 -> max 20 , symmetry=1 -> max 30
N_Y=N_X;
ASR_G=0.05; % ASR parametr, 1-no ASR, recommended value ~ 0.05


symmetry=1; % 1-yes, 2-no
symmetry_switch=5; % for theta!=0 -> use y-symmetry
% 1-x_symmetry_even
% 2-x_symmetry_odd
% 3-y_symmetry_even
% 4-y_symmetry_odd
% 5-x_y_symmetry_even_even
% 6-x_y_symmetry_odd_odd
% 7-x_y_symmetry_even_odd
% 8-x_y_symmetry_odd_even

diffaction_efficiency=[0,0]; % investigated diffraction orders (R,T)

input_file='coaxial_apertures_array.m';

measurement=3;
```

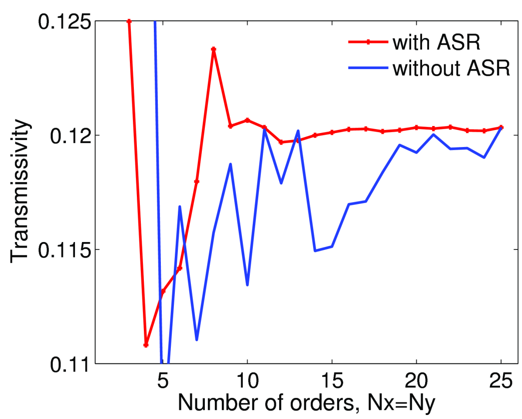


Figure 6: Convergence of order [0,0]

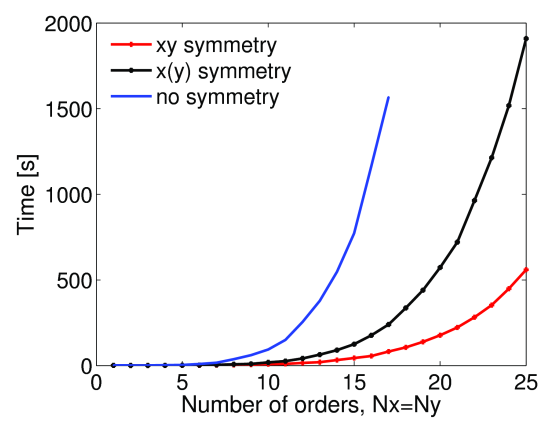


Figure 7: Comparison of computation times

The advantage of the ASR application is seen in Fig. 6 where the order [0,0] convergence with respect to the number of series-expansion terms included is shown. Also, Fig. 7 shows practically very important calculation time considerations, with a comparison of three cases: standard case with no symmetries, application of single symmetry only (x-axis), and simultaneous application of both symmetries (x and y-axis). The practical speed enhancement is clearly visible.

References to the ASR technique and application of structural symmetries in the RCWA method:

G. Granet, "Reformulation of the lamellar grating problem through the concept of adaptive spatial resolution," J. Opt. Soc. Am. A **16**, p. 2510, 1999

T. Vallius, M. Honkanen, "Reformulation of the Fourier modal method with adaptive spatial resolution: application to multilevel profiles," Opt. Express **10**, p. 24, 2002

Z. Y. Li, K. M. Ho, "Application of strucural symmetries in the plane-wave-based transfer-matrix method for 3D photonic crystal waveguides," Phys. Rev. B **68**, p. 245117, 2003

C. Zhou and L. Li,"Formulation of Fourier modal method of symmetric crossed gratings in symmetric mountings," J. Opt. A, Pure Appl. Opt. **6**, 43-50 (2004)