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# Analysis of crossed gratings with large periods and small feature sizes by stitching of the electromagnetic field

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We present a new algorithm that enables the analysis of large two dimensional optical gratings with very small feature sizes using the Fourier modal method. Which the conventional algorithm such structures cannot be solved due to limitations in computer memory and calculation time. By splitting the grating into several smaller sub-gratings and solving them sequentially, both memory requirement and calculation time can be reduced dramatically. We have calculated a grating with 32x32 pixels for a different number of sub-gratings. We show that the increased performance is directly related to the size of the sub-gratings. The field-stitched calculations proved to be very accurate and agree well with the predictions from the standard FMM approach. 

*OCIS codes:* 050.1755,050.1960,050.2770,350.3950

## 1. Introduction

Electromagnetic modelling of 3d volume gratings with sub wavelength feature sizes is extremely demanding both in computational time and memory. The Fourier modal method

(FMM) for crossed gratings [1–5] for example requires very high memory due to the large matrices that can easily exceed $10^7$ elements.

Many efforts have been undertaken to improve the convergence of the FMM in order to get reliable results with a lower number of Fourier orders. Bai and Li exploit symmetries of the investigated gratings [6–9]. Granet and Plumey introduced a parametric formulation of the FMM that increases the spatial sampling rates around discontinuities by means of a coordinate transform [10]. Schuster e.a. introduced a normal vector method in which a vector field is defined for each application to increase the convergence rate [11]. These methods however, are not feasible for large diffraction gratings with no symmetric features.



In this paper we introduce a field stitching method using the Fourier modal method for crossed gratings. This method is a generalisation of the 1d Field stitching method for lamellar gratings [12–14]. The large grating is split into several overlapping sub-gratings which can be solved separately. From the results of the sub-gratings, the global transmission and reflection coefficients can be calculated. The overlap of the sub-gratings ensures that no error is introduced at the edges from the new boundary conditions of each small grating as only the central part of the field will be taken into account.

In section 3 we derive the equations that connect the sub-gratings with the whole structure. The incident field for the sub-gratings as well as the transmitted and reflected field for the main grating are calculated.

In section 4 we show how rotation symmetries and mirror symmetries can be exploited to speed up the simulations. Sub-gratings that can be transformed into each other by a reflection or rotation only need to be solved once.

In section 5 we show numerical evidence of this method by analysing a 10x10 beam splitter consisting of 32 pixels in each direction.

## 2. Statement of the Problem

Consider a non magnetic crossed grating G with an arbitrary distribution of the permittivity $\epsilon(x, y)$. The grating can consist of several layers with $\epsilon(z)$ being constant in each of the layers. It is periodic in x and y with a large period $d_x$ and $d_y$ compared to the features within the grating and a thickness $t$ which should be small in respect to $d_x$ and $d_y$. The grating divides two homogeneous semi infinite half spaces $R_1$ $(z < 0)$ and $R_2$ $(z > h)$ with refractive index $n_1$ and $n_2$ respectively. The electromagnetic field in $R_1$ and $R_2$ can be decomposed as a series of plane waves. Inside the grating the field is expressed by a superposition of Floquet modes which are found with the FMM. To connect the field of $R_1$ with $R_2$ a scattering matrix $\mathbf{S}$ of the grating is calculated. A monochromatic linearly polarised light from $R_1$ with vacuum wavelength $\lambda$ and an incident angle $\theta$ to the z-axis and $\phi$ to the x-axis respectively illuminates the grating.

If the grating does not scatter light strongly into the xy-plane, only areas in the immediate neighbourhood influence the field at each point in the grating. In the following sections we will use this property to split the problem of a single large grating to several problems of small sub-gratings.



## 3. 2d Field Stitching Method

### A. Representation of the external field with the FMM

In the FMM the electromagnetic field is represented by Floquet modes. In region $R_1$ and $R_2$ (before and after the element) the field can be written as a Rayleigh expansion:

$$E^1_\sigma = \sum_{mn} (I_{\sigma,mn} + R_{\sigma,mn}) \times \exp\left[i(\alpha_m x + \beta_n y + \gamma^{-1}_{mn})\right] \quad (1)$$

$$E_\sigma^2 = \sum_{mn} T_{\sigma,mn} \exp\left[i(\alpha_m x + \beta_n y + \gamma_{mn}^1)\right] \tag{2}$$

with $\alpha_m = k_x^{+1} + m2\pi/d_x$, $\beta_n = k_y^{+1} + n2\pi/d_y$, $\gamma_{mn}^{(a)} = (k^{(a)2} - \alpha_m^2 - \beta_n^2)^{1/2}$. $\sigma$ is the polarisation of the electric field and can be either x or y. $I_{\sigma,mn}$ are the Fourier coefficients of the transmitted light, $I_{\sigma,mn}$ are the coefficients of the incident light and $R_{\sigma,mn}$ for the reflected light respectively.

To calculate the field propagation of an element large in size with many, very small features, a very high number of Raleigh orders is required to get a accurate representation of the field as well as for the refractive index in the grating. The computational cost increases dramatically with the number of Raleigh orders which pushes even very modern computers to their limits.



### *B. Derivation of the transmission and reflection modes*

The grating is divided into N adjacent rectangular regions (see Fig. 6). Each of the regions is extended in x and y direction to ensure that all areas of the grating that influence the field at the edges are included (see Fig.6). For the calculation of the transmission and reflection orders of the whole grating only the central part of the field of each sub-grating will be taken into account. To simplify the calculations each sub-grating has a coordinate system attached to it with the origin in the lower left corner. The transformation from the global coordinate system to the coordinate system of the sub-gratings is denoted by the translation vector $\mathbf{r}_n$.

The origin of the coordinate system of sub-grating n is

$$\mathbf{r}^n = (x_1^n - x_s^n, y_1^n - y_s^n, 0) \tag{3}$$

where $(x_n, y_n)$ is the lower left corner of the non overlapping part of the grating, $x_s^n$ and $y_s^n$ are the overlap in x and y direction. The size of sub-grating n is

$$\begin{aligned} d_x^n &= (x_2^n + x_s^n) - (x_1^n - x_s^n) \\ d_y^n &= (y_2^n + y_s^n) - (y_1^n - y_s^n) \end{aligned} \tag{4}$$

where $x_2^n$ and $y_2^n$ is the upper limit of the non overlapping area.

The spatial frequencies in the computational cell are

$$\mathbf{k}_{pq} = (\alpha_p, \beta_q) \tag{5}$$

$$= (\alpha_0 + 2\pi p d_x^{-1}, \beta_0 + 2\pi q d_y^{-1}) \tag{6}$$

for the large grating and



$$\mathbf{k}_{pq}^n = (\alpha_0^n + 2\pi p (d_x^n)^{-1}, \beta_0^n + 2\pi q (d_y^n)^{-1}) \tag{7}$$

for the sub-gratings.

The transform of the electric and magnetic field between the coordinate systems is

$$U_n(\mathbf{r}) = U(\mathbf{r} + \mathbf{r}_n) \tag{8}$$

where $\mathbf{r}$ defines the position within the sub-region, $U_n$ is the electric or magnetic field representation in respect to the sub-area and $U$ is the field representation in respect to the whole element.

The field in the n$^{th}$ subregion can be expressed as a Fourier expansion for both the sub-region and the whole grating which both have to give the same result. We use equation (8) to calculate the incident modes of each sub region. By putting the Fourier expansion of the incident field into (8) we get

$$\sum_{pq} I_{pq}^n \exp\left(i\mathbf{k}_{pq}^n \mathbf{r}\right) = \underbrace{\sum_{st} I_{st} \exp\left(i\mathbf{k}_{st} \cdot (\mathbf{r} + \mathbf{r}_n)\right)}_{=f(\mathbf{r})} \tag{9}$$

which has the form of a discrete Fourier transform with the Fourier coefficients $I_{pq}^n$ which can be calculated by

$$
\begin{aligned}
I_{pq}^n &= (d_x^n d_y^n)^{-1} \int_0^{d_x^n} \int_0^{d_y^n} f(\mathbf{r}) \exp\left(-i\mathbf{k}_{pq}^n \mathbf{r}\right) \mathrm{dxdy} \\
&= (d_x^n d_y^n)^{-1} \textstyle\sum_{st} I_{st} \exp\left(i\mathbf{k}_{st}\mathbf{r}^n\right) \\
&\quad \times \int_0^{d_x^n} \int_0^{d_y^n} \exp\left(i(\mathbf{k}_{st} - \mathbf{k}_{pq}^n)\mathbf{r}\right) \mathrm{dxdy}
\end{aligned} \tag{10}
$$

The reflection and transmission orders can be calculated as a combination of the sub-regions in a similar way by using the reverse translation relation between the coordinate systems:



$$
U(\mathbf{r}) = U_n(\mathbf{r} - \mathbf{r}_n) \qquad \begin{cases} x_1^n < x < x_2^n \\ y_1^n < y < y_2^n \end{cases} \tag{11}
$$

For this calculation it is important to choose the correct sub-region which contains $\mathbf{r}$.

Putting the Fourier expansion of the reflected and transmitted field into equation (11) we can identify the transmission and reflection modes as coefficients of a discrete Fourier transform which are calculated by

$$
\sum_{pq} T_{pq} \exp\left(i\mathbf{k}_{pq}\mathbf{r}\right) = \underbrace{\sum_{st} T_{st}^n \exp\left(i\mathbf{k}_{st}^n(\mathbf{r} - \mathbf{r}^n)\right)}_{=f(\mathbf{r})} \tag{12}
$$

and

$$
\sum_{pq} (R_{pq} + I_{pq}) \exp\left(i\mathbf{k}_{pq}\mathbf{r}\right) = \underbrace{\sum_{st} (R_{st}^n + I_{st}^n) \exp\left(i\mathbf{k}_{st}^n(\mathbf{r} - \mathbf{r}^n)\right)}_{=f(\mathbf{r})} \tag{13}
$$

The coefficients $T_{pq}$ and $R_{pq}$ can be calculated in the same manner as the $I_{pq}^n$ in equation

10.

$$T_{st} = (d_x d_y)^{-1} \sum_{pq} T^n_{pq} \exp\left(i\mathbf{k}^n_{pq}\mathbf{r}^n\right) \times \int_0^{d_x}\int_0^{d_y} \exp\left(i(\mathbf{k}^n_{pq} - \mathbf{k}_{st})\mathbf{r}\right) \mathrm{dxdy} \quad (14)$$

In this equation the parameters of the correct sub-grating have to be chosen according to x and y in the integral. Thus the integral has to be broken up into a sum of N integrals - one for each sub-grating - to get the right coefficients for each point of the structure:



$$T_{st} = (d_x d_y)^{-1} \sum_{n}\sum_{pq} T^n_{pq} \exp\left(i\mathbf{k}^n_{pq}\mathbf{r}^n\right) \times \int_{x_1^n}^{x_2^n}\int_{y_1^n}^{y_2^n} \exp\left(i(\mathbf{k}^n_{pq} - \mathbf{k}_{st})\mathbf{r}\right) \mathrm{dxdy} \quad (15)$$

and

$$(R_{st} + I_{st}) = (d_x d_y)^{-1} \sum_{n}\sum_{pq} (R^n_{pq} + I^n_{pq}) \exp\left(i\mathbf{k}^n_{pq}\mathbf{r}_n\right) \times \int_{x_1^n}^{x_2^n}\int_{y_1^n}^{y_2^n} \exp\left(i(\mathbf{k}^n_{pq} - \mathbf{k}_{st})\mathbf{r}\right) \mathrm{dxdy}\ . \quad (16)$$

### *C. Special case: Small modulated area in black surrounding*

In order to calculate the far-field of of an isolated element, the periodic effects of the transmitted field have to be reduced. This can be done by embedding the structure in a large non-emitting padding so that light of diffracted orders reach the boundary farther away from the element. By choosing an appropriate size of the padding, it is possible to remove the interference effects for the region of interest. We have introduced this method for lamellar gratings [15]. Here we show a generalisation to 2 dimensional gratings. The new Fourier orders for the larger area can be calculated using the above introduced field stitching method:

$$T_{st} = (d_x d_y)^{-1} \sum_{pq} T'_{pq} \exp\left(i\mathbf{k}'_{pq}\mathbf{r}'\right) \times \int_{x_1}^{x_2} \int_{y_1}^{y_2} \exp\left(i(\mathbf{k}'_{pq} - \mathbf{k}_{st})\mathbf{r}\right) \mathrm{dxdy} \quad (17)$$



$d_x$ and $d_y$ are the dimensions of the larger area with spatial vectors $\mathbf{k}_{pq}$. The primed variables refer to the small coordinate system of the element. The coordinates of the lower left and upper right corner of the element are $(x_1, y_1)$ and $(x_2, y_2)$ respectively.

## 4. Exploiting Symmetries of the Structure for Field Stitching

If the structure to be investigated shows mirror symmetry (C2 or C4) or rotational symmetry (SO2 or SO4) each group of symmetric sub-gratings only need to be solved once. The transmission coefficients of the symmetric partners can be calculated with coordinate transformations. The field is written generally as $U^{(n)}(x, y)$ with the corresponding Fourier coefficients $X^{(n)}_{pq}$. The field U can be substituted with the reflected, transmitted and incident field. For the ease of reading, $\mathbf{k}_{pq}$, and $d_x$ and $d_y$ are defined as the parameters of the sub-gratings in quadrant 1. For the following calculations we assume the grating to be illuminated from $R_2$ with an incident angle of $\theta = 0$.

The calculation of the transmitted and reflected field involves many coordinate transforms of the vectors containing the Fourier coefficients of the electric field. The field vectors containing the Fourier coefficients are transformed in a way that the calculated field is mirrored or rotated by multiples of 90°. When using the FMM with a square truncation scheme and truncation order M, the Field vectors have $2N^2$ elements, $N^2$ for x-polarisation and $N^2$

for y-polarisation with N=2M+1. The elements of the vector are defined by 3 indices (see equations (1) and (2)):

$$X_{\sigma mn} = X_{\sigma N^2+mN+n} \tag{18}$$

where $\sigma$ is 0 for x-polarisation and 1 for y-polarisation respectively. m and n go from 0 to N denoting the coefficients from -M to +M.

If the grating has C4 mirror symmetry (Fig. 6(a)), the transformation of the field in region 1 to regions 2, 3 and 4 are:



$$U^{(2)}(x, y) = U^{(1)}(x, -y) \tag{19}$$

$$U^{(3)}(x, y) = U^{(1)}(-x, -y) \tag{20}$$

$$U^{(4)}(x, y) = U^{(1)}(-x, y) \quad . \tag{21}$$

For SO4 rotational symmetry (Fig. 6(b)) we get:

$$U^{(2)}(x, y) = U^{(1)}(y, -x) \tag{22}$$

$$U^{(3)}(x, y) = U^{(1)}(-x, -y) \tag{23}$$

$$U^{(4)}(x, y) = U^{(1)}(-y, x) \tag{24}$$

To get an equation for the Fourier coefficients we substitute the Fourier series of the field in the original sub-grating and the symmetric sub-grating into equations (19) to (24)

With the incident angle of the light being normal to the grating surface, i.e. $\theta = 0$, we can simplify equation 25. In this case we get $\alpha_0 = \beta_0 = 0$, $\alpha_m = -\alpha_{-m}$ and $\beta_m = -\beta_{-m}$. The field in region 2 of Fig. 6(b) is calculated from the field in region 1 with the relation

$$\begin{aligned} U^{(2)}(x,y) &= \frac{1}{d_x d_y}\sum_{pq} X^{(2)}_{pq}\exp\left(i(\alpha_p x+\beta_q y)\right) \\ &= \frac{1}{d_x d_y}\sum_{pq} X^{(1)}_{pq}\exp\left(i(\alpha_p x+\beta_q(-y))\right) \\ &= \frac{1}{d_x d_y}\sum_{pq} X^{(1)}_{p,-q}\exp\left(i(\alpha_p x+\beta_q y)\right) \end{aligned} \tag{25}$$

so

$$\sum_{pq}(X^{(2)}_{pq}-X^{(1)}_{p,-q})\exp\left(i\mathbf{kr}\right)=0 \quad . \tag{26}$$



The exponential functions in (26) form a set of orthogonal functions so the coefficients of each $\exp(i\mathbf{kr})$ must add to 0.

We now have an equation for $X^{(2)}_{p,q}$:

$$X^{(2)}_{p,q}=X^{(1)}_{-p,q} \quad . \tag{27}$$

Regions 3 and 4 are solved the same way:

$$X^{(3)}_{pq}=X^{(1)}_{-p,-q} \tag{28}$$

$$X^{(4)}_{pq}=X^{(1)}_{-p,q} \quad . \tag{29}$$

For a S04 symmetry the shape of the sub-gratings must be quadratic which means $\alpha_p=\beta_p$. The relations are then

$$X^{(2)}_{pq}=X^{(1)}_{q,-p} \tag{30}$$

$$X^{(3)}_{pq}=X^{(1)}_{-p,-q} \tag{31}$$

$$X^{(4)}_{pq}=X^{(1)}_{-q,p} \tag{32}$$

We define a transform $\mathcal{C}$ that defines how to swap the elements in the field vectors according to (27)-(32):

$$\mathcal{C}_{b,a}(X_{\sigma,m,n}) = X_{\sigma,n,m} \tag{33}$$

$$\mathcal{C}_{a,-b}(X_{\sigma,m,n}) = X_{\sigma,m,-n} \tag{34}$$

$\mathcal{C}_{-a,b}$, $\mathcal{C}_{-a,-b}$ and $\mathcal{C}_{-b,-a}$ are defined likewise. $\mathcal{C}_{a,b}$ is the identity.

In the following sections we describe how to calculate the field vector of the transmitted field for sub-gratings with a symmetric partner. The calculations for the reflected field are identical, to get the equations the $T$ is substituted by $R$.



### A. *Plane wave incident field*

If the incident light is just a plane wave, all sub-gratings have the same incident field which is invariant to rotations and reflections. The easiest way to get the field vector of the transmitted field in regions 2 to 4 is by applying the appropriate transform $\mathcal{C}$ to the T vectors of region 1.

$$\mathbf{T^{(n)}} = \mathcal{C}(\mathbf{T^{(1)}}) \tag{35}$$

### B. *Exploiting symmetry for a spatially structured incident beam*

If the incident light is not a plane wave but has a certain phase and amplitude distribution the method described above cannot be applied because sub-gratings from different parts of the grating will have a different field. The transmission coefficients can then not be calculated by a simple permutation rule. However it is still possible to obtain the transmission orders of symmetric sub-gratings as the scattering matrix of symmetric gratings are equivalent. In this case the calculation consists of three steps:

Firstly, the incident field of the sub-grating to solve needs to be transformed to the coordinate system of the already solved sub-grating. The incident field is transformed by

$$\mathbf{I^{(n)}} = \mathcal{C}(\mathbf{I^{(1)}}) \tag{36}$$

Secondly, the transmission coefficients are calculated by multiplying the transformed incident field vector $I'$ with the scattering matrix S of the sub-grating in region 1: plying $I'$ with the scattering matrix S of the sub-grating in region 1:

$$\mathbf{T}' = \mathbf{S} \cdot \mathbf{I}' \tag{37}$$



In the last step the transmission field vector $T'$ is transformed back to the orientation of the symmetric grating with the same transform as in step 1.



$$\mathbf{T^{(n)}} = \mathcal{C}(\mathbf{T}') \tag{38}$$

Combining all steps into one concise equation gives

$$\mathbf{T^{(n)}} = \mathcal{C}(\mathbf{S^{(1)}} \cdot \mathcal{C}(\mathbf{I^{(n)}})) \tag{39}$$

## 5. Numerical performance

The underlying principle of the Field stitching method is to increase the spatial resolution of the discrete Fourier transform not by increasing the number of Fourier orders but to decrease the period of the computational cell. If, for example, a grating of size $d_x \times d_y$ is solved using a truncation order N, the maximum spatial frequency in x is $\alpha_{max} = 2\pi m/d_x$. If the grating is split into $a \times a$ sub-gratings and each grating is solved individually with a truncation order N, the maximum spatial frequency in x is

$$\alpha'_{max} = 2\pi m/(d_x/a) = a\alpha_{max} \tag{40}$$

This means for the same spatial resolution the matrices used in the calculation of the scattering matrix are much smaller. The increase of the spatial resolution is directly proportional to the decrease of the size of the sub-gratings. We can define an effective truncation order $N_{eff}$that corresponds to the truncation order of the standard FMM approach. For a grating that is split in $a \times a$ regular parts, the effective truncation order is

$$N_{eff} = aN \tag{41}$$

For a square truncation scheme with truncation order N the S-Matrix has a size of $(2N^2)^2$. Figure 6 shows the required memory of the S-Matrix. Each element of the matrix is complex with double precision which takes 16byte of memory.



Based on the theory presented above, a computer program was built to test the numerical performance. The diffractive phase grating in figure 6 was solved with the Fourier modal method. As a reference the whole structure was solved. For the field stitching method the grating was split up into a regular grid of 2x2 and 4x4 sub-gratings. The grating parameters are $n_1 = n_2 = 1$, $\theta = \phi = 0°$, $h = 2\lambda$, $d_1 = d_2 = 32\lambda$. Each pixel in the grating is quadratic with side length $\lambda$.

Figure 6 shows the convergence of the three different transmission orders as a function of the effective truncation order. For the FMM calculations a quadratic truncation scheme was used. Using the field stitching method the convergence of the result can be improved a lot which means a much larger grating could be solved without increasing the memory requirement as each sub-grating is solved sequentially. This diagram also provides evidence to the use of an effective truncation order. The lines using 2 by 2 sub-gratings as well as 4 by 4 sub-gratings match nearly exactly the line for the standard FMM approach.

Figure 6 shows the calculation time for solving the grating in figure 6 as a function of the effective truncation order. The calculations were performed using computer with two Intel Xeon 3000 double core processors with a clock speed of 3GHz. The computation time difference between the standard approach and the 4x4 field stitching approach is more than two orders of magnitude.

This example shows that for large thin gratings the Field stitching method for crossed gratings reduces the memory requirements as well as the calculation time. If a grating shows symmetries, the calculation time is reduced by a further factor of 2 for C2 and SO2 symmetry and a factor of 4 for C4 and S04 symmetry respectively as each group of symmetric sub-gratings only needs to be solved once.

## 6. Conclusion



We introduced a generalisation of the Field stitching method to crossed gratings. The relation between the transmission and reflection coefficients of the sub-gratings and the main grating were derived. For a further improvement of the Field stitching method we exploited properties of gratings that show mirror symmetric or discrete rotational symmetric properties. On an example of a diffractive element that acts as a 10 by 10 beam splitter we showed the numerical performance of the Field stitching method. Both memory requirements and calculation time can be reduced by orders of magnitude. This method can be used not only for the Fourier modal method but for all modal methods such as the method of moments (MOM) or the rigorous coupled wave analysis (RCWA).

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**List of Figures**

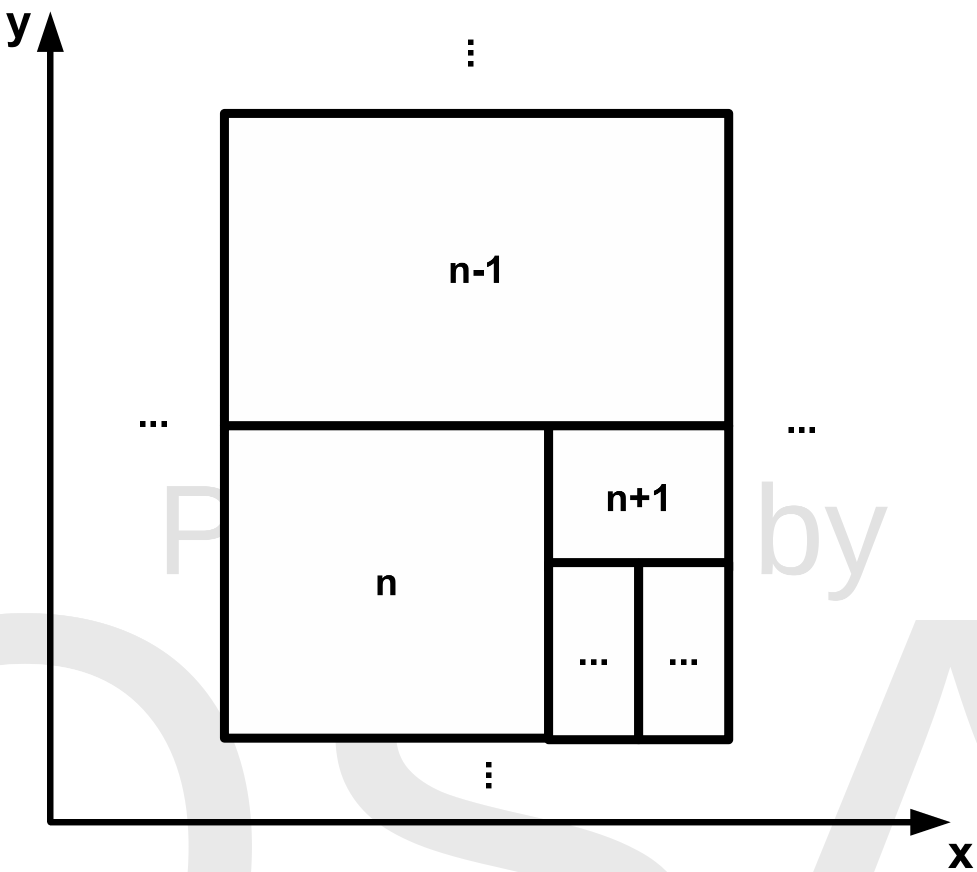




Fig. 1. The grating is split up into adjacent rectangular sub-gratings numbered from 1 to N. They do not necessarily have to have the same size and shape.

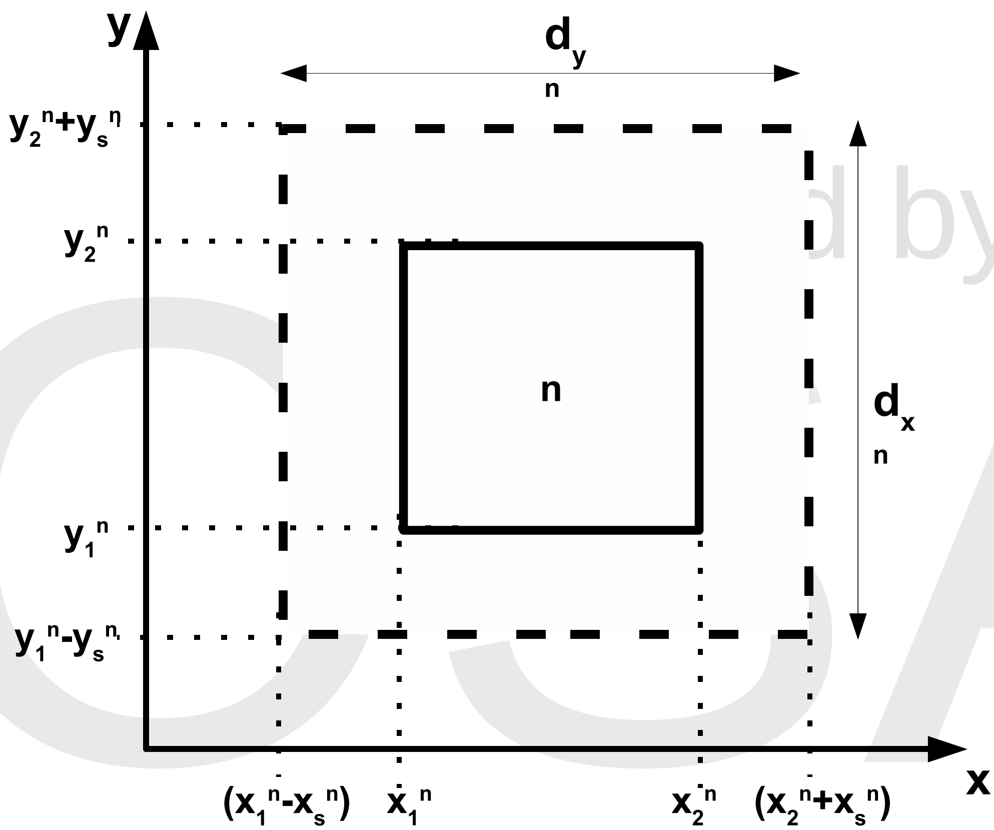


Fig. 2. Each sub-grating is extended by a frame with dimension $x_s$ and $y_s$. This ensures that the field at the edges are calculated correctly

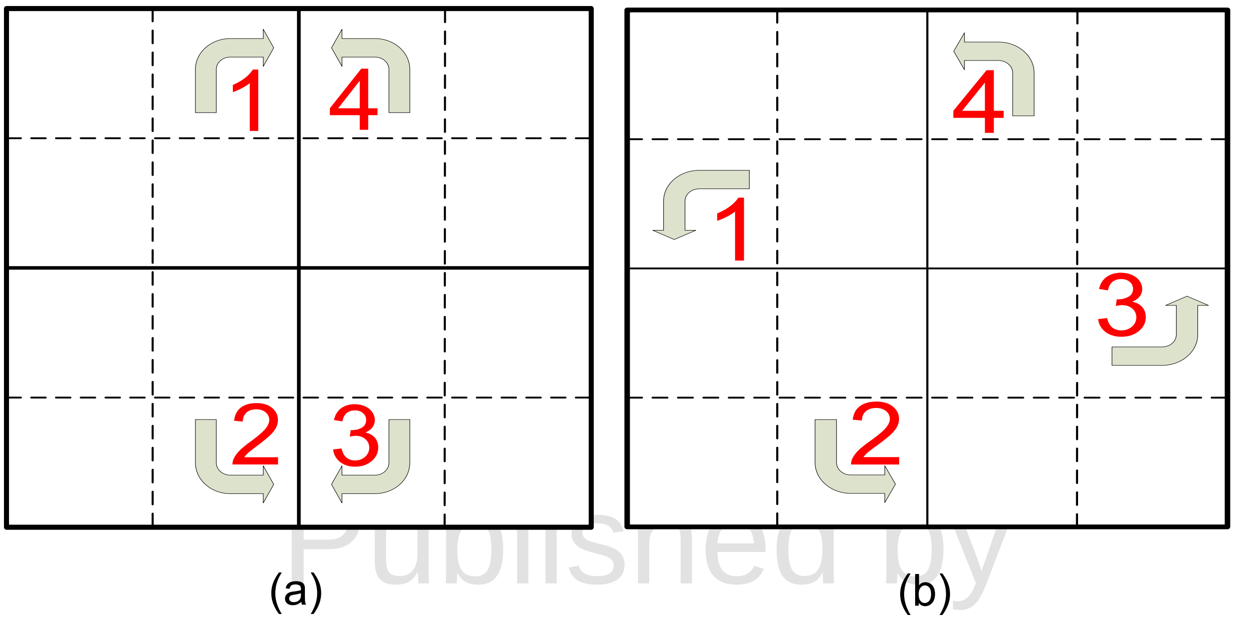




Fig. 3. Sub-gratings that can be transformed into each each other by reflection (left) or rotation (right) only need to be solve once. The transmission coefficients and reflection coefficients for all partners can easily be calculated

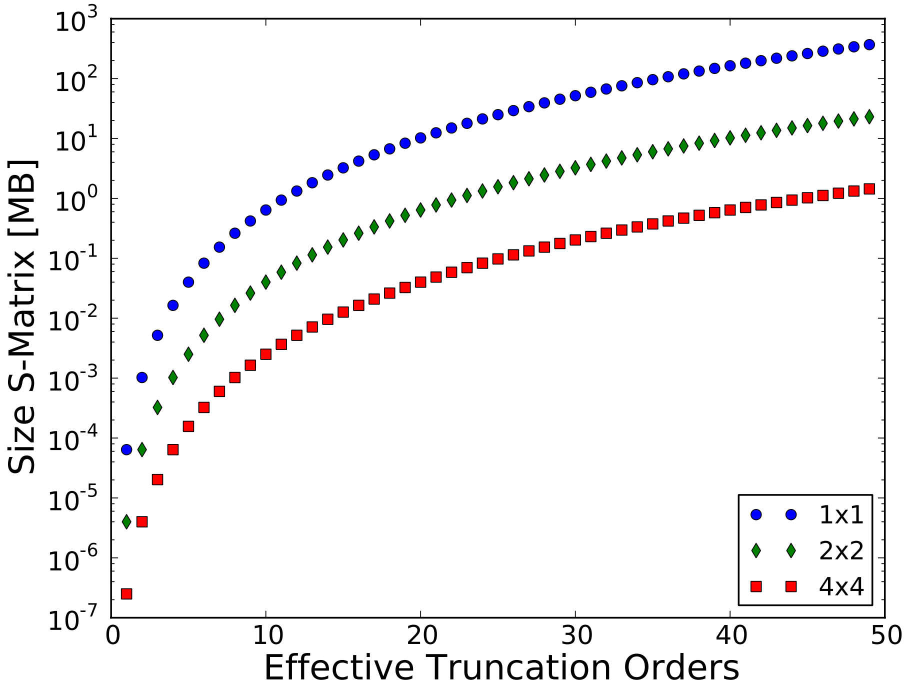


Fig. 4. The size of the S-Matrix as a function of the effective truncation order

2

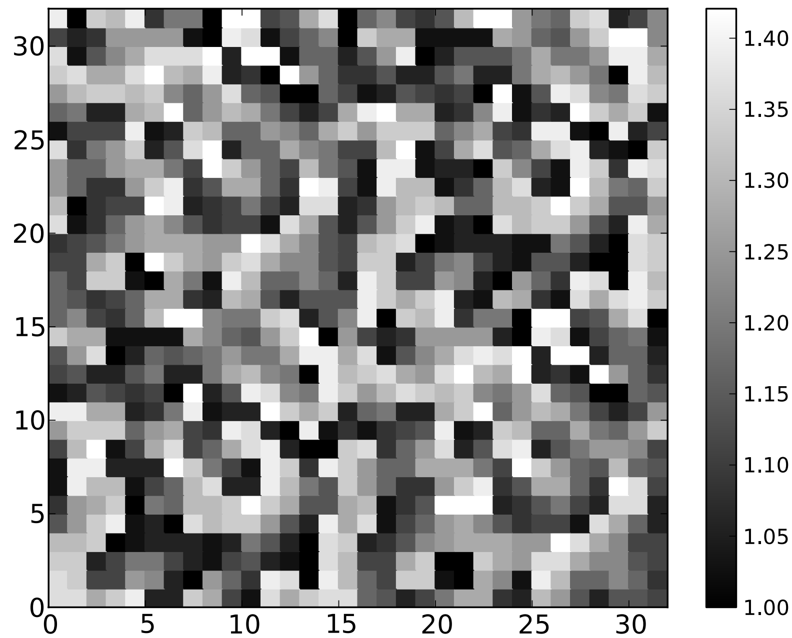


Fig. 5. Diffractive phase grating designed as 10x10 beam splitter. The grating consists of 32x32 pixels and 7 refractive index levels

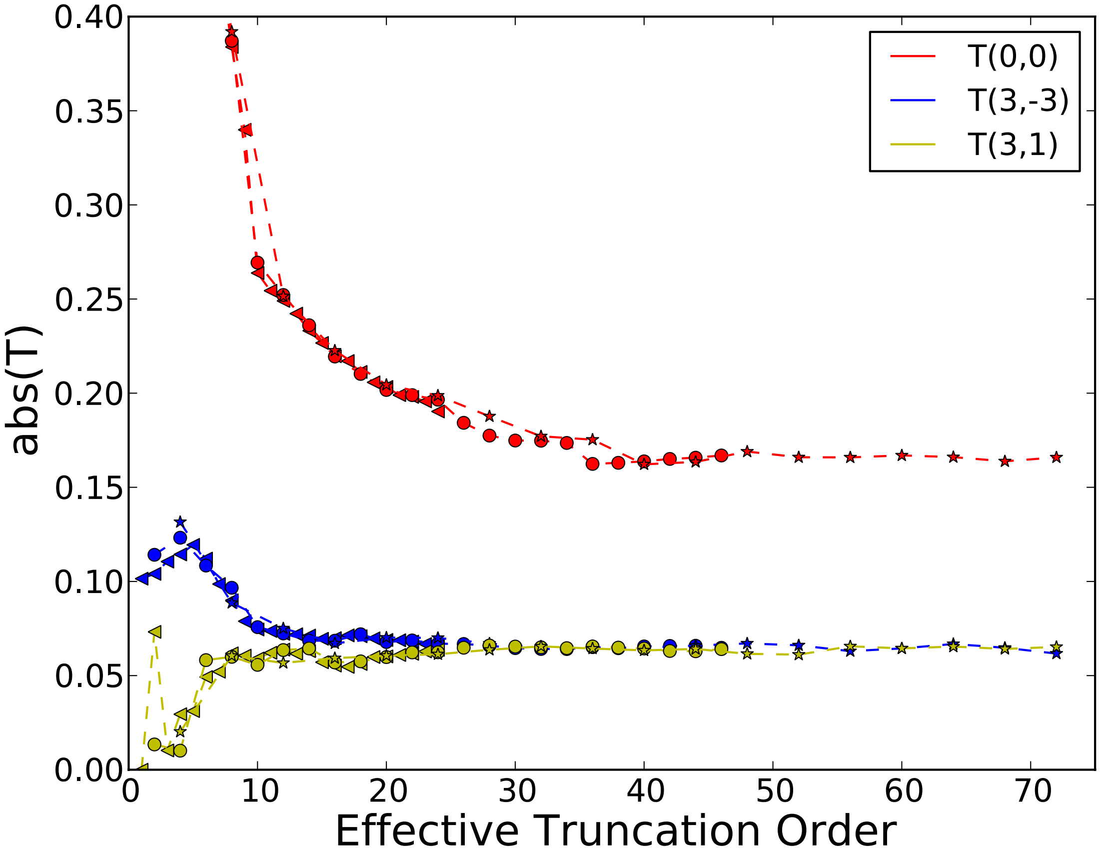


Fig. 6. The convergence of the absolute value of three transmission orders. All three cases show the convergence for the standard FMM approach (triangle) and for the field stitching algorithm with 2x2 sub-gratings (circle) and 4x4 sub-gratings (star).

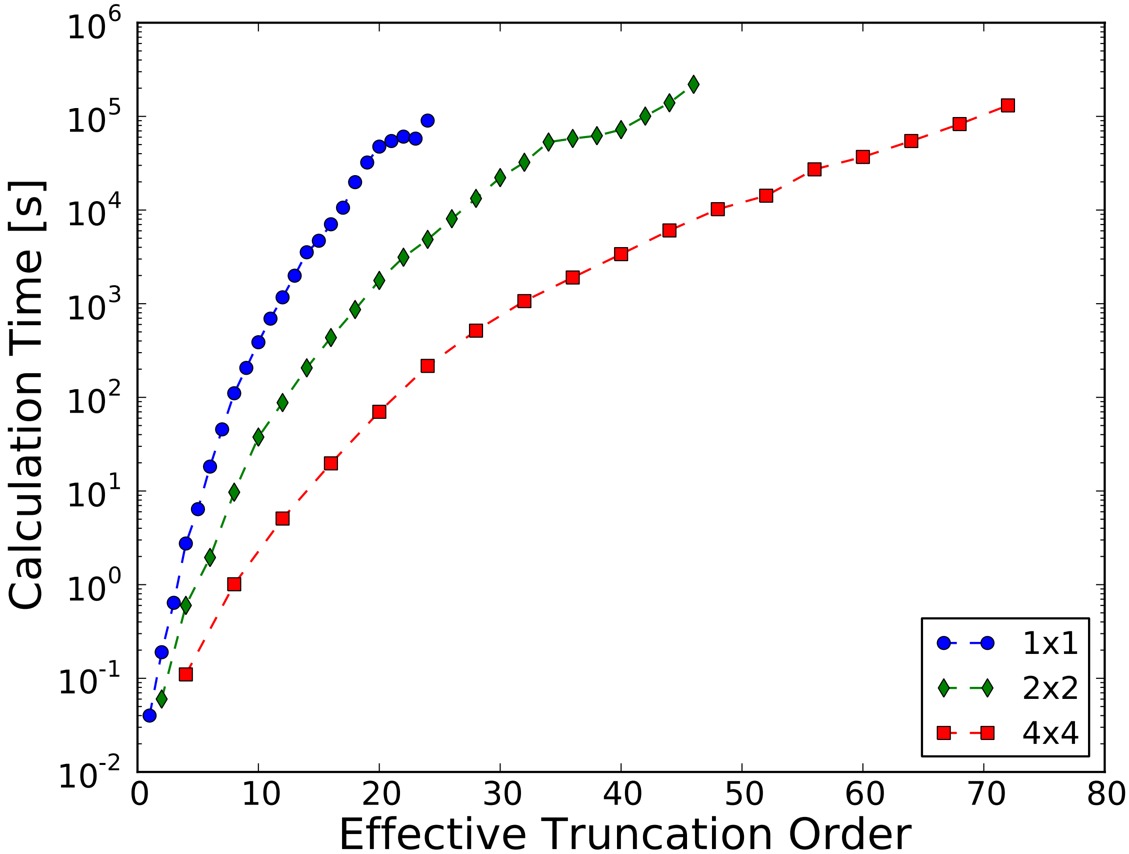


Fig. 7. The calculation time as a function of the effective truncation order. The green line shows the trend for the undivided structure, the red and blue line show the trend for a 2x2 division and 4x4 division respectively