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THE LAMELLAR DIFFRACTION GRATING PROBLEM : A SPECTRAL METHOD BASED ON SPLINE EXPANSION

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Abstract. Our aim is to solve the electromagnetic problem of the diffraction of a plane wave by a one dimensional lamellar grating. In that case the solution to Maxwell's equations can be split into two canonical cases : the so-called transverse magnetic (TM) and transverse electric (TE) polarizations. These cases can be treated separately, reducing the problem to a scalar one. In this paper we only consider the TE polarization case in which the only non null component of the electric field is parallel to the grating grooves. Since the grating is invariant in one direction the Maxwell's equations reduce to an eigenvalue problem for which a numerical solution is obtained by using the method of moments. First the unknown function is expanded in a series of spline functions and then the operator deduced from the Maxwell's equations is projected onto a set of test functions after a suitable inner product has been defined. The choice of the basis and test functions and their properties have an essential impact for the rate of convergence. One of the reasons for choosing splines functions is that they were successfully used in the signal processing field.

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We can take advantage of their analytical definition as piecewise polynomials and their compact support. Concerning the test functions, we compare three possible choices : Dirac, gate or spline functions. Thanks to their attractive properties, these functions allow calculating analytically the matrix coefficients deduced from the inner product. The computational effort is therefore drastically minimized.

1. Introduction

The scale of microelectronic devices continues to decrease. At smaller scales, the relative impact of intrinsic circuit properties such as interconnections may become more significant. The goal of the microelectronics is to find ways to compensate for or to minimize these effects, while always delivering smaller, faster, and cheaper devices.

Many applications in microelectronics fields require the electromagnetic equations to be modeled accurately within a very short computation time. To manufacture advanced integrated circuits optical projection micro lithography is used and pushed very close to the physical resolution limits. The correction of the so called optical proximity effects at the mask level is a mandatory step. This requires fully optimized models and a fast and accurate solution of the electromagnetic problem is required.

Many rigorous methods exist but large efforts remain to be made on obtaining 3D electromagnetic codes that are sufficiently robust and fast. The finite difference (FD) modal method and the coupled-wave method [1] also called the Fourier modal method (FMM) are examples of the most efficient and commonly used methods to solve diffraction problems.

On the other hand, in the field of signal processing, functions with a compact support showed a very strong potential through their ability to provide fast convergence. We used the spline expansion to solve the 2D electromagnetic problems that appear in several lithography applications to improve the efficiency of the current methods based on a modal approach. The improvement is obtained thanks to a rigorous numerical treatment of the discontinuities of the permittivity function.

2. Definition of the problem

2.1. **Physical formulation.** We consider the case of a lamellar grating configuration as shown in fig.1.

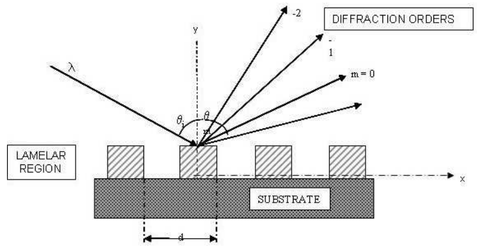

FIGURE 1. Geometry of the diffraction problem

A piecewise homogenous medium is characterized by a refractive index that is periodic along the x direction with a d period.

$$\nu_2(x) = \begin{cases} \nu_{21} & \text{for} \quad 0 \leq x \leq fd \\ \\ \nu_{22} & \text{for} \quad fd \leq x \leq d \end{cases} \tag{1}$$

where f is a parameter between 0 and 1.

The refractive index of the medium through which the light is incident is denoted by ν_1 and that of the substrate ν_3. These refractive indices may be complex, describing lossy dielectrics or metals with the exception of the incident medium which is assumed to be vacuum. This structure is illuminated by a linearly polarized monochromatic plane wave. The wave is inclined at $\theta°$ on the $0y$ axis. Our goal is to determine the ratio of the diffracted light intensity, of a given diffracted order, to the incident light intensity namely the reflected and transmitted diffraction efficiencies.

2.2. **Mathematical formulation.** This paragraph outlines the mathematical approach of the physical problem presented above. In order to describe the properties of the electromagnetic field, the Maxwell equations are solved in a Cartesian coordinate system (x, y, z). It can be shown that the electromagnetic field can be expressed as sum of a transverse electric (TE) and transverse magnetic (TM) polarization part. In the TE polarization case the only nonzero components are (H_x, H_y, E_z) while in TM polarization the only nonzero components are (E_x, E_y, H_z). Both polarizations can be treated separately, reducing the problem to a scalar problem. For the sake of simplicity we treat only the TE polarization case. Then for a time dependance of the form $e^{i\omega t}$, Maxwell's equations write:

$$\begin{cases} \partial_y E_z = -i\omega\mu_0 H_x \\ \\ \partial_x E_z = i\omega\mu_0 H_y \\ \\ \partial_x H_y - \partial_y H_x = i\omega\epsilon_j(x) E_z \end{cases} \tag{2}$$

where $\partial_x = \frac{\partial}{\partial_x}$ and $\epsilon_j\left(x\right) = \nu_j^2\left(x\right)$ characterizes the lamellar grating permittivity , $j = \{1, 2, 3\}$. Eliminating H_x and H_y in equation (2) the propagation equation is obtained:

$$\left(\frac{1}{k^2}\partial_x^2 + \epsilon_j(x)\right) E_z\left(x, y\right) = -\frac{1}{k^2}\partial_y^2 E_z\left(x, y\right) \tag{3}$$

where $k = \frac{2\pi}{\lambda}$ is the wavenumber (λ =wavelength). Since the operator at the left-hand side of the equation (3) depends only on x-variable, the solution can be expressed as:

$$E_z(x, y) = f(x)e^{\pm ikry}$$

Thus an eigenvalue problem is obtained:

$$\mathcal{L}f(x) = r^2 f(x) \tag{4}$$

where $f(x)$ and r^2 are the eigenfunction and eigenvalues respectively, $\mathcal{L}$ is a linear operator that depends only on the x-variable.

$$\mathcal{L} = \frac{1}{k^2}\frac{d^2}{dx^2} + \epsilon_j(x)$$

The square root of the eigenvalue is chosen so that the propagative wave amplitude decreases along the propagation direction so only the eigenvalues that fulfill the following condition are selected :

$$r \in \mathbf{R}^+ \text{ or } r \in \mathbf{C} \text{ and } Im\left(r\right) < 0$$

The boundary conditions at the interfaces of the three regions determine the amplitude field coefficients. The field E_z may be expanded in an eigenfunction series:

$$E_z(x, y) = \sum_{m=1}^{\infty}(A_m^+ e^{ikr_m y} + A_m^- e^{-ikr_m y}) f_m(x) \tag{5}$$

where A_m^+ and A_m^- denote the upward and downward field amplitude. The diffracted and refracted efficiencies are then expressed as:

$$R_n = \frac{r_{1n}}{r_0} A_{1n}^+ (A_{1n}^+)^* \quad T_n = \frac{r_{3n}}{r_0} A_{1n}^- (A_{1n}^-)^*$$

where the subscript n refers to the n^{th} reflected or transmitted order, whilst the subscript 0 refer to the incident wave.

2.3. **Numerical approach.** In this paragraph, the details for the numerical implementations are presented. Equation (4) is reduced to a matrix form and solved using the method of moments [2]. This consist into two steps. Firstly, each f_m from equation (5) is expanded into a finite weighted sum of basis functions B_n. Secondly, this expansion is projected onto a set of test functions T_q. We denote by N the truncation number, all the indexes are assumed by default $\{1, 2, ...N\}$. Equation (3) leads to the following matrix form:

$$\left[\mathbf{G}^{-1}\left(\mathbf{D}\mathbf{G}^{-1}\mathbf{D} + \mathbf{G}^{\epsilon}\right)\right][E_{z_n}] = r^2 [E_{z_n}] \tag{6}$$

where $\mathbf{G}$, $\mathbf{D}$ are square matrix expressing the inner product between the test functions and the basis functions as well as the inner product between the test function and the derivative of the basis function respectively.

$$\mathbf{G} = [\langle T_q, B_n \rangle] \quad \mathbf{D} = \left[\left\langle T_q, B_n^{'} \right\rangle\right] \tag{7}$$

The matrix $\mathbf{G}^{\epsilon}$ takes into account the jump of the permittivity function :

$$\mathbf{G}^{\epsilon} = [\langle T_q, \epsilon B_n \rangle] \tag{8}$$

2.4. **Adaptive spatial resolution.** In order to improve the numerical results, an adaptive spatial resolution is implemented [1]. For that purpose, a new system of coordinates (u, y, z) is introduced. $x(u)$ is chosen so that the spatial resolution increases around the $x = 0$ and $x = fd$, points where the permittivity function is discontinuous. The following function is used :

$$x = \begin{cases} u - \eta \frac{f}{2\pi} \sin\left(\frac{2\pi u}{fd}\right) \text{ if } u < fd \\ \\ u + \eta \frac{1-f}{2\pi} \sin\left(\frac{2\pi(d-u)}{(1-f)d}\right) \text{ if } u \le d \end{cases} \tag{9}$$

where η is a parameter between 0 and 1.

A short computation shows that only the matrix $\mathbf{D}$ from the equation (6) is changed into $\dot{X}\mathbf{D}$, where $\dot{X}$ is a square sparse matrix containing the values of the derivative of the $x(u)$ function on its main diagonal.

3. Spline expansion

The basis functions used in this paper are the splines of the second order defined as in ref. [3]. As the above problem is pseudoperiodic, the basis functions used must be periodic. This condition is accomplished by the first ϕ_1 and the last ϕ_N splines. The figure below shows the example of spline functions over the interval $[0, 1]$. One can see that the first and the last spline assure the periodicity.

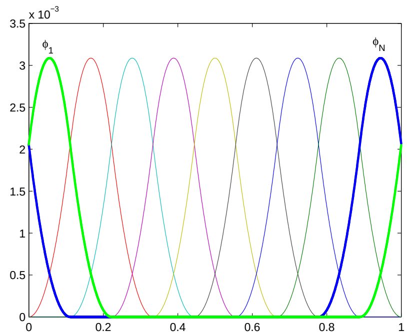

Figure 2. Spline functions. The first and the last spline function are drawn with bold lines

In order to take into account the pseudoperiodicity properties of the field, a phase factor is added to the periodic basis functions ϕ_n :

$$B_n = e^{(-ik_0\alpha_0 x)}\phi_n(x) \qquad \text{with } \alpha_0 = sin(\theta_0)$$

The support of the basis functions B_n remains compact due to the compactness of the support of the spline function ϕ_n.

4. Test Functions

The inner product involved into evaluation of the operator from the equations (7) and (8) is often difficult to perform in problems of practical interest.

A simple way to obtain approximate solutions is to require that equation (6) be satisfied for a discrete set of points in the region of interest. This procedure is called a point-matching method. In terms of the method of moments, it is equivalent to using Dirac delta functions as test functions. These points are denoted by $x_n = n\dfrac{d}{N}$ where $n = \{0, 1, ..., N-1\}$.

Another approach for this practical problem of diffraction is to use a gate function as test function. A possible definition of a gate function is detailed below :

$$\sqcap_{n,N}(x) = \begin{cases} \frac{9}{4N}\left(\frac{d}{N}\right)^2 & x \in [x_n, x_{n+1}] \\ \\ 0 & \text{otherwise} \end{cases} \tag{10}$$

Finally, another particular choice of test functions is known as Galerkin's method. More precisely, in this kind of approach the test functions are identical to basis functions : $T_q = B_q$.

The evaluation of the matrix coefficients of $\mathbf{G}$, $\mathbf{D}$ and $\mathbf{G}^{\epsilon}$ from the equation (6) involves time consuming numerical integrations. These matrices contain inner products of the form $\langle T_q, B_n\rangle$ so an integration must be computed. Even though the integration limits range from 0 to d, the intervals of actual integrations are much smaller because of the compact support of the test and basis functions. By taking advantage of this property many entries of the matrices can be directly identified to zero. Only these inner products in which the test and the basis functions overlap, have to be computed.

5. Illustration of the results

We model the impact of a grating on a TE polarized incident wave. We consider the same grating geometry previously studied by Lalanne [4] ($d = 1\mu m, f = 0,5\mu m, h = 1\mu m, \lambda = 1\mu m, \nu_{22} = \nu_3 = 0.22 - 6.71 * i$, and $\theta = 30°$). The figure 3 shows the zeroth order reflected diffraction efficiency computed with spline basis functions projected on the Dirac, gate or spline functions as test functions as a function of the truncation order. For the sake of comparison the results obtained with FD modal method taken from Ref.[4] are also plotted.

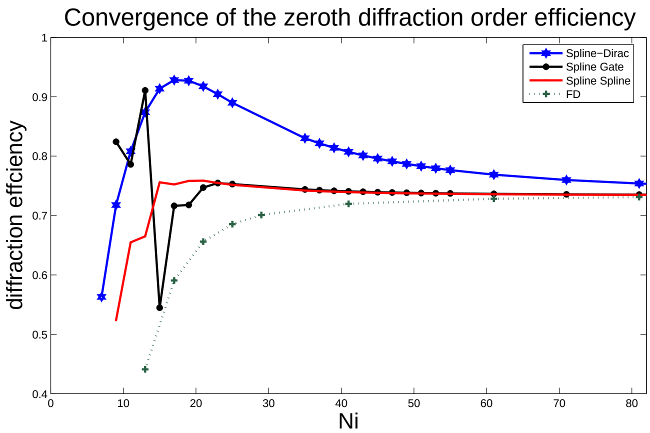

FIGURE 3. Comparison of different implementations of different methods

It is seen that the gate-spline (stars) and the Galerkin's method (dotted line) results compares favorably with the Finite Difference-modal method. As could be expected the Galerkin's method gives us the most accurate results.

6. Conclusion

In this paper, we solved Maxwell's equations with a modal method. Numerically, the solution of the eigenvalue problem is obtained by using the method of moments : the unknown function is expanded on a set of basis functions and equations are projected on a set of test functions. This approach was also used in the finite difference modal method. The fundamental difference between the latter and our approach is the choice of the basis and test functions.

In our method, the splines were chosen as basis functions whereas the FD-modal method uses gate functions. The FD-modal method uses the Dirac functions as test functions. For the sake of comparison, we have introduced three test functions: the Dirac(point matching method), gate and spline functions(Galerkins method). On the case investigated in this paper the rate of convergence of the FD-modal, gate-spline and Galerkin's methods, are comparable. Our three approaches of the diffraction problem allow us to conclude that the more elaborate the test functions, the more accurate the results.

Another strong point is that splines allow calculating the inner product analytically. Furthermore, this method offers symmetrical sparse matrices. The computational effort and the space memory are therefore drastically minimized.

Other numerical simulations not presented in this paper show that numerical results obtained with our approach converge slightly slower than those given by the adaptive spatial resolution Fourier modal method, at least on the specific example considered here. We may conclude that on this specific case, the convergence speed places it between the adaptive FMM and non-uniform sampling FD-modal method.

This paper is the starting point for the wavelets splines and multiresolution analysis. The addition of a hierarchical basis will allow the implementation of a multilevel analysis, preferably located around a region of the field with rapid variation. Thus, the use of a spline expansion will certainly provide better performance than the Fourier Modal Method. This next step of our work will be presented in a subsequent paper.

References

[1] G. Granet, **Reformulation of the lamellar grating problem through the concept of adaptive spatial resolution**, J.Opt.Soc.Am./ Vol **16** (2510-2516), October 1999.

[2] R. Harrington, **Field computation by Moment Methods**, New York: The Macmillan 1968.

[3] K. Edee, P. Schiavone and G. Granet, **Analysis of defect in extreme UV Lithography mask using a modal method based on nodal B-spline expansion**, Japanese Journal of Applied Physics/ Vol **44**.No 9A, (6458-6462),2005.

[4] P. Lalane and J.P Hugonin, **Numerical performance of finite-difference Modal Method for the electromagnetic analysis of one-dimensional grating**, J.Opt.Soc.Am./ Vol **17**.No 6: June 2000.

[5] R. Harrington, **Matrix Methods for Field Problem**, Proceeding of the IEEE Vol.55. No 2: page 136-149, February 1967.

[6] Ph. Lalane and G. M. Morris, **Highly improved convergence of the coupled-wave method for TM polarization**, J.Opt.Soc. Am. A **13**, 779-784 (1996).

[7] G. Granet and B. Guizal, **Efficient implementation of the coupled-wave method for metallic lamellar gratings in TM polarization**, J.Opt.Soc. Am. A **13**, 1019-1023 (1996).

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