Light diffraction on metal gratings under conical incidence by the true-mode method

Ivan Gushchin, Alexander V. Tishchenko and Olivier Parriaux

Laboratoire Hubert Curien, UMR 5516 Université Jean Monnet-CNRS, 42000 Saint Etienne, France
E-mail: tishchen@univ-st-etienne.fr

Abstract. A microstructured metallic surface gives rise to a number of interesting visual effects which can advantageously be used is security elements. The modeling of such effects is still an open issue as far as 1D periodic structures under conical incidence and 2D structures are considered. The true-mode method has the potential of becoming a reference method for such difficult electromagnetic problems. This was already demonstrated in 1D gratings under collinear incidence. It will soon be demonstrated in the case of 2D metallic gratings. On the way to this objective we are reporting here on the implementation of the true-mode method for conical incidence on 1D-metal gratings.

1. Introduction
Most anti-counterfeit structures of the diffractive type make use of three basis materials: at least one polymer for the substrate and the cover layer, one high index material to boost the diffraction effects, usually ZnS, and a metal layer, usually aluminum, to enhance the diffraction efficiency and permit a visualization of the encoded picture in reflection. The present need for increasingly secure features leads to more complex diffraction effects such as resonant mechanisms involving 2D periodic structures and arbitrary incidence conditions. Such complex diffraction conditions in the presence of a metal still represents big hurdles for electromagnetic theory and modeling. Whereas the manufacturing technologies already exist for fabricating such microstructures, the modeling techniques lag behind and there is a need for a fast and accurate method capable of solving 2D diffraction problems involving metallic parts. We are developing further the “true-mode method” which was shown to be a reference method for 1D metallic gratings. Before addressing the full 2D problem we are here reporting on the true-mode method applied to conical diffraction on 1D dielectric and metal gratings.

2. Problem formulation
Diffraction grating and system configurations are depicted in Figure 1.

A monochromatic plane wave with frequency \( \omega \) falls from semi-infinite media I with permittivity \( \varepsilon_I \) and permeability \( \mu_I \) on the grating at polar angle and azimuthal angle. Field expression would be in the form:

\[
E' \exp(ik_x x + ik_y y - ik_z z - i\omega t)
\]  

(1)
where \( k_i = \omega \sqrt{\varepsilon_i \mu_i} \), \( k_x = k \sin(\theta) \cos(\phi) \), \( k_y = -k \sin(\theta) \sin(\phi) \) and \( k_z = k \cos(\theta) \). Time dependence in the form \( \exp(-i\omega t) \) for all solutions of Maxwell’s equations is assumed and suppressed for brevity throughout the paper. Semi-infinite region II below the grating is with permittivity \( \varepsilon_{II} \) and permeability \( \mu_{II} \). Period of the grating is \( d \) along \( x \)-direction. We will use the following definition of polarization in semi-infinite media for conical mount (Figure 2).

**Figure 1.** Diffraction grating configuration

We would call a plane TE-polarized, when magnetic field lays in the plane of incidence; and TM-polarized when electric field lays in this plane. As positive direction of vectors would be taken direction on the right from plane of incidence. So, it’s possible to define all field components using this plane wave amplitudes definition and taking Maxwell’s equations into account.

It becomes impossible to define polarization when incidence at angle \( \theta = 0 \) with such definition of TE and TM projection, but this situation is already solved in the non-conical mount.

Resulting field, produced by diffraction of a plane wave on a periodic structure may be presented as a sum of diffracted plane waves (in the form of Rayleigh expansion). The fields under and above grating can be expressed in the following way:

\[
\begin{bmatrix}
E_j \\
H_j
\end{bmatrix} = \sum_{m=-\infty}^{\infty} \begin{bmatrix}
\gamma^m_j & -i\omega_j m \\
-i\omega_j m & \gamma^m_j
\end{bmatrix} \exp\left[ik_j^m(z - z_j)\right] + \begin{bmatrix}
\gamma^m_j & i\omega_j m \\
-i\omega_j m & \gamma^m_j
\end{bmatrix} \exp\left[-ik_j^m(z - z_j)\right] \exp\left(ik_j^mx + ik_jy\right) \tag{2}
\]

where \( j \) — number of semi-infinite media and \( m \)-order number in Rayleigh-Fourier expansion and

\[
k_j^m = \sqrt{\omega^2 \varepsilon_j \mu_j - (\gamma_j^m)^2}, \quad \left(\gamma_j^m\right)^2 = \left(k_j^m\right)^2 + \left(k_j^y\right)^2.
\]

The solution of the diffraction problem is conventionally represented by the S matrix relating all the diffracted wave amplitudes to the incident wave amplitudes. Finding such bound between wave amplitudes is very useful for numerical calculations of the stack of such periodical obstacles or in slicing method that is used with modal method calculations.

### 3. Modal Method

We would use modal method for representing field in grating region. Grating is infinite in \( y,z \)-directions and periodical in the \( x \) direction. \( d \) is the period of the grating in sense that functions \( \varepsilon(x), \mu(x) \) satisfies condition \( f(x+d) = f(x) \). Modes are field solutions satisfying quasi-periodicity condition.
Inside the grating region we would call mode TE-polarized in case \( E_x=0 \), and TM-polarized in case \( H_x=0 \). It’s shown in literature [1], that in non-conical mount for infinite in 2 directions grating: 1) solutions may be separated for TE and TM polarization 2) there exist propagation constants \( \beta^a_q \) (where \( a \) – polarization and \( q \) – number of mode) along plane of infinite directions for each polarization. Field distribution function along x-axes \( \psi^a_q(x) \) exists for each of propagation constants. Field distribution function and its propagation constant are bound by following equation, depending on polarization:

\[
\begin{bmatrix}
\psi^a_q(x) \\
\chi^{a*}(x)
\end{bmatrix}' + \left[ \omega^2 \varepsilon(x) \mu(x) - \left( \beta^a_q \right)^2 \right] \begin{bmatrix}
\psi^a_q(x) \\
\chi^{a*}(x)
\end{bmatrix} = 0, \quad a = e, h, \quad \chi^e(x) = \mu(x), \quad \chi^h(x) = \varepsilon(x)
\] (4)

where \( \psi^a_q(x) \) is eigenfunction, describing field distribution along x-axis for \( a \) polarization, \( \beta^a_q \) is eigenvalue for this eigenfunction. Another functional basis can be build, such that \( \bar{\beta}^a_q = \beta^a_q \) and

\[
\frac{1}{d} \int_{0}^{d} \frac{\psi^a_q(x) \psi^{a*}_{q'}(x)}{\omega \chi^{a*}(x)} dx = \delta_{pq},
\]

where “plus” means complex conjugate, overline denoting eigenfunctions and eigenvalues of the following equation:

\[
\begin{bmatrix}
\psi^a_q(x) \\
\chi^{a*}(x)
\end{bmatrix}' + \left[ \omega^2 \varepsilon^+(x) \mu^+(x) - \left( \beta^a_q \right)^2 \right] \frac{\psi^a_q(x)}{\chi^{a*}(x)} = 0
\] (5)

These two bases are bi-orthogonal that allows representing any function in the form:

\[
F(x) = \sum_{q=0}^{\infty} A_q \psi^a_q(x)
\] (6)

where \( A_q = \frac{1}{d} \int_{0}^{d} F(x) \frac{\psi^a_q(x)}{\omega \chi^a(x)} dx \) - coefficient for \( q \)-th mode (polarisation notes are suppressed, as they have no influence on equations view).

Conical mount differs from classical mount in \( k_y \neq 0 \), but field distribution of each mode with propagation constant \( \beta \) in x-direction remains the same. That is unlike classical mount when field is propagated in one direction with full propagation constant in conical mount part of the propagation constant is already defined with \( k_y \). That is we may write \( \left( \beta^a_q \right)^2 = k^2_y + (k^a_{zy})^2 \) where \( k_y \) is projection of falling wave vector (defined in previous section), and \( k^a_{zy} \) is propagation constant in z-direction (up or down) for a given polarization and mode number. Full field presentation as a superposition of all modes existing in grating.

4. Rectangular profile

This modal field representation is obtained from assumption of infinity in z-direction and exists as field solution in grating region. For grating of a finite depth same field representation can be used, i.e.
if exists some complete basis of solutions in an infinite grating, then in a finite grating one solution would be represented by the same basis. Thus, we represent the field in semi-infinite media as a superposition of diffracted waves and in the grating region as a superposition of grating modes.

We consider a plane interface parallel to the XY plane. Boundary conditions at the interfaces are:

\[ E_{x \text{ semi}} = E_{x \text{ grating}} \quad H_{x \text{ semi}} = H_{x \text{ grating}} \]
\[ E_{y \text{ semi}} = E_{y \text{ grating}} \quad H_{y \text{ semi}} = H_{y \text{ grating}} \]

Substituting expressions for each field component in the homogeneous media and in the grating region we get the system of equations:

\[ E_x : \sum_{q=-\infty}^{\infty} \left( \frac{\beta_q}{\omega \varepsilon} \psi_q^+(x) \left( a_q^+ + a_q^- \right) \right) = \sum_{m=-\infty}^{\infty} \left( \frac{k}{\varepsilon_m} \left( b_m^+ + b_m^- \right) \exp(ik_m^+ \cdot x) \right) + \sum_{m=-\infty}^{\infty} \left( -\frac{k}{\varepsilon_m} \frac{k}{\varepsilon_m} \left( b_m^+ - b_m^- \right) \exp(ik_m^+ \cdot x) \right) \]
\[ E_y : \sum_{q=-\infty}^{\infty} \left( \frac{\beta_q}{\omega \mu} \psi_q^+(x) \left( a_q^+ - a_q^- \right) \right) = \sum_{m=-\infty}^{\infty} \left( \frac{k}{\mu_m} \frac{k}{\mu_m} \left( b_m^+ - b_m^- \right) \exp(ik_m^+ \cdot x) \right) + \sum_{m=-\infty}^{\infty} \left( \frac{k}{\mu_m} \left( b_m^+ + b_m^- \right) \exp(ik_m^+ \cdot x) \right) \]
\[ H_x : \sum_{q=-\infty}^{\infty} \left( \frac{\beta_q}{\omega \mu} \psi_q^+(x) \left( a_q^+ + a_q^- \right) \right) = \sum_{m=-\infty}^{\infty} \left( \frac{k}{\mu_m} \frac{k}{\mu_m} \left( b_m^+ - b_m^- \right) \exp(ik_m^+ \cdot x) \right) + \sum_{m=-\infty}^{\infty} \left( \frac{k}{\mu_m} \left( b_m^+ + b_m^- \right) \exp(ik_m^+ \cdot x) \right) \]
\[ H_y : \sum_{q=-\infty}^{\infty} \left( -\frac{i k}{\omega \mu} \psi_q^+(x) \left( a_q^+ - a_q^- \right) \right) = \sum_{m=-\infty}^{\infty} \left( \frac{k}{\mu_m} \frac{k}{\mu_m} \left( b_m^+ - b_m^- \right) \exp(ik_m^+ \cdot x) \right) + \sum_{m=-\infty}^{\infty} \left( -\frac{k}{\mu_m} \left( b_m^+ + b_m^- \right) \exp(ik_m^+ \cdot x) \right) \]

The transition matrix is a matrix that bounds field amplitudes at one side of the interface with those at the other side. Matrix expression in the form \( \mathbf{B} = \mathbf{T} \mathbf{B}' \) can be obtained in two different ways.

The first method, which seems to be the easiest way is to multiply the left and right parts by \( \exp(-ik_m^+ x) \), then, integrate over one period. This procedure leads to obtaining system of equations in the form:

\[ \sum_{q=0}^{\infty} \text{INTEGRAL}_q a_q^{z,e,h} = \text{coefficients} \cdot b_m^{z,e,h} \]

where we have \( 4N \) equations on \( 4N \) variables (b-set) defined by the infinite sum of another set of variables (a-set). Resolving this system we get the following matrix form:

\[
\begin{pmatrix}
\left( b^+ \right) \\
\left( b^- \right) \\
\left( b^h \right) \\
\left( b^-h \right)
\end{pmatrix}
= 
\begin{pmatrix}
\left( T^{+e} \right) \\
\left( T^{-e} \right) \\
\left( T^{+h} \right) \\
\left( T^{-h} \right)
\end{pmatrix}
\begin{pmatrix}
\left( a^{+e} \right) \\
\left( a^{-e} \right) \\
\left( a^{+h} \right) \\
\left( a^{-h} \right)
\end{pmatrix}
\]

In the infinite equation system, each component is considered as an infinite vector. Such matrix expressions are already well known.

Multiplying the right side by an exponential can be considered as calculating the Pointing vector, or in another words, calculating energy propagation expressed in the left and in the right sides.

Pointing vector expresses the energy propagating in given direction:
\[ S = \frac{\text{Re}(E \times H^*)}{2} \]  

(10)

It represents power propagated by the field superposition but also it equals to the sum of powers transported by each mode in upward and downward directions:

\[
\int_{0}^{d} S_{z} \, dx = \int_{0}^{d} E_{x} H_{y}^{*} - E_{y} H_{x}^{*} \, dx = \int_{0}^{d} \left( \sum_{q} E_{xq} \sum_{p} H_{yp}^{*} - \sum_{q} E_{yq} \sum_{p} H_{xp}^{*} \right) \, dx = \sum_{q} \int_{0}^{d} E_{xq} H_{yq}^{*} - E_{yq} H_{xq}^{*} \, dx \]  

(11)

This approach plays an important role in obtaining a matrix which is opposite to the previous one: \( T \downarrow \rightarrow \bar{T} \). As a test function we choose TE- or TM- mode. The field projections in the expression of \( S_{z} \) are replaced by this test function. Thus, we obtain four equations:

\[
\begin{align*}
\hat{E}_{xq}^e \sum_{p} H_{yp}^e - \hat{E}_{yq}^e \sum_{p} H_{xp}^e &= S_{q}^z \\
\hat{E}_{xq}^h \sum_{p} H_{yp}^h - \hat{E}_{yq}^h \sum_{p} H_{xp}^h &= S_{q}^z \\
\sum_{p} E_{xp} \times H_{yp}^e - \sum_{p} E_{yp} \times H_{xp}^h &= S_{q}^z \\
\sum_{p} E_{xp} \times H_{yp}^h - \sum_{p} E_{yp} \times H_{xp}^e &= S_{q}^z
\end{align*} \]  

(12)

where the “tilde” denotes a complementary test function, \( q \) is the mode number, polarization is denoted by letters \( e \) or \( h \).

After integrating over one period and using that field functions are periodical we get

\[
\int_{0}^{d} S_{q}^z \, dx = C(a_{q}^{+p} \pm a_{q}^{-p}) \]  

(13)

Calculating each equation in such manner leads to the system of linear equations from which the matrix coefficients can be easily retrieved. Finally, the \( S \) matrix can be found from the \( T \) matrix using the algorithm described in [2].

5. Numerical Results

We have used this approach to calculate diffraction efficiencies dependence on azimuthal angle. In all calculations was used polar angle of 37°, wavelength 652.6 nm, binary grating of half-wavelength groove depth, line/period ratio 0.5 with air as the second medium. The groove index was chosen \( n=0.14 + i \times 4.15 \) (metal). Substrate of the grating is of the same material as grating. Dependence of different reflection efficiencies into TE polarization versus azimuthal angle for dielectric grating and for TM diffraction into TM are shown in Fig. 3. Similar dependence on line/period ratio is represented in Fig. 4. Azimuthal angle was equal 20°.

6. Conclusion

Expressing transition matrix components allows receiving solutions both for dielectric grating and for metal grating. This technique can also be used to express field amplitudes excited by incident wave inside the grating.

The true-mode method has here been extended to 1D periodic structures possibly involving metallic parts under conical incidence conditions. The electromagnetic problems which have been
solved are also those which will be encountered in the exact modelling of 2D metallic gratings by means of the modal method. It is believed that such approach will offer a fast and exact representation of all effects produced by increasingly complex security features.

**Figure 3.** Dependence of reflection efficiencies of different orders on the angle of incidence

**Figure 4.** Reflection efficiency as a function of duty cycle of a binary grating

**References**

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[2]  Tishchenko AV 2005 *Optical and Quantum Electronics* **37**:1-3 309-30