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Metody analýzy difrakčních mřížek a jejich využití

Methods of diffraction grating analysis and their applications

SUMMARY

The presentation describes the problem of analysis of optical diffraction gratings and its possibilities for application to selected types of diffractive and optical structures. This is, in fact, the complex research field covering the problems from diffractive optics, through general optics and electrodynamics, numerical modeling, up to linkage to respective design, synthesis, practical realization and specific applications.

In the first part of this presentation, the brief overview of the optical diffraction grating analysis is given, the basic diffraction problem is formulated, and the terminology used is introduced. The viewpoint is such that diffraction gratings form the most significant part of more general optical diffractive structures. Their analysis is thus highly needful; and understandably, in many applications the elementary picture, based on Fourier optics, is not sufficient. The attention must hence be given also to more general pictures. Approaches to grating analysis, resulting from the diffraction problem formulation, can be divided to rigorous and approximate ones.

The second part is devoted to a brief description of the two selected rigorous methods (rigorous coupled wave analysis, coordinate transformation method) and one special approximate method of grating analysis (effective medium theory applicable to high spatial frequency gratings) which have been studied in detail. The basic idea and algorithm of each method are shown, together with its implementation, usage and application possibilities; the methods are also compared to each other and our contribution is pointed out.

Next part concentrates on our original results and demonstrates feasibility of utilization of analysis methods, using both results from modeling of general diffraction characteristics (characteristic regions of diffraction, volume phase synchronism) and results on selected problems which have been dealt with (resonant effects in gratings, realistic grating diffraction efficiency modeling, modeling of high spatial frequency structure characteristics, grating waveguide couplers, structures of photonic crystals, and discussion of analysis as a part of the design process).

Hence, we will attempt to demonstrate how applications of the analysis methods for optical diffraction gratings open up new possibilities in many branches of diffractive (and more generally applied) optics, especially for design and realization of practically interesting optical structures.

In the field of grating analysis, several rigorous and approximate methods have been developed, implemented and employed. On several selected examples, their applicability and usage for different modeling problems (not only from the field of diffractive optics) will be shown. Finally, the overview of implemented methods and modeling results is given and main conclusions and contributions of presented activities for further research work and teaching activities in the field are brought together, along with future outlooks.

SOUHRN

Prezentace popisuje problematiku analýzy optických difrakčních mřížek a možnosti její aplikace na vybrané typy difraktivních a optických struktur. Jedná se o komplexní problematiku zahrnující problémy z difraktivní optiky, přes obecnou optiku, elektrodynamiku a numerické modelování až po vazbu na vlastní návrh, syntézu, praktickou realizaci a konkrétní aplikační využití.

V první části této prezentace bude uveden stručný přehled problematiky analýzy optických difrakčních mřížek, bude formulován základní difrakční problém a uvedena používaná terminologie. Úhel pohledu je přitom takový, že difrakční mřížky tvoří nejvýznamnější součást obecnějších optických difraktivních struktur. Jejich analýza je proto velmi potřebná, v mnoha aplikacích se přitom pochopitelně nevystačí s elementárním pohledem, vycházejícím z fourierovské optiky, ale je třeba věnovat pozornost i pohledům obecnějším. Možnosti přístupů k analýze mřížek vyplývající z formulace difrakčního problému je možno rozdělit na rigorózní a přibližné.

Druhá část je věnována podrobnějšímu pohledu na dvě vybrané metody rigorózní (rigorózní metoda vázaných vln, metoda transformace souřadnic) a jednu speciální metodu přibližnou (metoda efektivního prostředí aplikovatelná na vysokofrekvenční mřížky), kterými jsme se detailně zabývali. Je vždy ukázána základní myšlenka a algoritmus metody, její implementace, použití a aplikační možnosti, s důrazem na náš vlastní přínos, provedeno je také srovnání přístupů.

V další části jsou, s využitím vlastních originálních výsledků, ukázány možnosti aplikací metod analýzy, jednak na výsledcích z oblasti modelování obecných difrakčních charakteristik (charakteristické oblasti difrakce, objemový fázový synchronizmus), jednak na vybraných problémech, kterými jsme se zabývali (rezonanční jevy v mřížkách, modelování difrakční účinnosti reálných mřížek, modelování vlastností vysokofrekvenčních struktur, mřížkové vazební členy, struktury fotonických krystalů, diskuze analýzy jako součásti procesu návrhu).

Pokusíme se tím demonstrovat, jak aplikace metod analýzy optických difrakčních mřížek otevírá nové možnosti v mnoha odvětvích difraktivní (a obecněji aplikované) optiky, zejména pro návrh a realizaci aplikačně zajímavých optických struktur. V oblasti analýzy difrakčních mřížek bylo vyvinuto, implementováno a aplikačně využíváno několik rigorózních i přibližných metod. Na příkladech bude ukázána jejich aplikovatelnost a využití pro modelování problémů, nejen z oblasti difraktivní optiky. Závěrem je uveden přehled vytvořených metod a výsledků modelování a jsou shrnuty přínosy prezentované práce pro další výzkumné i pedagogické aktivity v této oblasti, spolu s dalšími výhledy.

Keywords: optical diffraction gratings, diffractive structure, high spatial frequency structure, diffractive optics, rigorous grating analysis, rigorous coupled wave analysis, coordinate transformation method, effective medium theory, volume phase synchronism, resonant effect, guided mode resonance filter, grating coupler, photonic crystal, photonic band gap

Klíčová slova: optická difrakční mřížka, difraktivní struktura, vysokofrekvenční struktura, difraktivní optika, rigorózní analýza mřížek, rigorózní metoda vázaných vln, metoda transformace souřadnic, metoda efektivního prostředí, objemový fázový synchronismus, rezonanční efekt, vlnovodný rezonanční filtr, mřížkový vazební člen, fotonický crystal, fotonický zakázaný pás

CONTENTS

1. INTRODUCTION

Today, ***optical diffractive structures*** (ODS) including periodic grating structures represent very perspective elements of modern optics. Extensive applications of diffractive structures cover nowadays such distinct areas as optical security and counterfeiting, display holography, measuring techniques and interferometry, high-power laser technologies, spectroscopy, through utilization in general optics, integrated optics, sensors, up to optical information processing, optical interconnects and optical computing [1-4]. Such structures possess specific characteristics and features, especially a capability of arbitrary general optical signal transformations and processing. Field of ODS, including analysis, design, synthesis, and optimization, together with realization technology, hence have established the new area of diffractive optics. ODS are considered as optical periodic or quasiperiodic microstructural systems with a material parameter modulation; optical wave is then formed on such structures via diffraction process. For such formation, quantization of phase levels is typically used which transforms both amplitude and phase in a desired manner.

As a special case, ***optical diffraction gratings*** (ODG) represent periodically modulated structures (with a periodicity Λ, grating vector $\vec{K}$) [5,6]. From a viewpoint of optical wave formation, such a grating can be formed through quantization of above mentioned phase levels applied to linear function. Basic classification of ODG (and also ODS), based on a relation of Λ and wavelength of light, gives low-frequency, medium-frequency, and high frequency structures; traditionally the last two being the subject of diffractive optics research. Research on both ODG and ODS represents a complex activity, reaching from analysis, through synthesis (design), technological methods of realization, characterization, and testing, up to final application exploitation. For the purpose of this presentation, the analysis problem is of interest.

There are several classification criteria of gratings, depending on their dimensionality, type and shape of modulation, thickness of a grating region, type of a grating material, etc. The modulation itself is typically realized either via direct dielectric permittivity (refractive index) modulation, or via indirect modulation – through surface-relief corrugation.

Thus, the ***analysis*** of behavior and detailed modeling ***of diffraction gratings*** represent an important part of the process which importance has even increased recently due to a rise of new synthetic technologies of realization (e.g., lithographic direct and mask techniques) [7-9]. Obviously, it is also important for analysis and design considerations of more general ODS. In a narrower sense, considered also mainly in this contribution, grating analysis represents a process of finding diffraction efficiencies of real diffraction orders, based on grating and incident wave parameters. As a multiparameter problem, even in a simplest case, the diffraction on a grating depends on many grating parameters (period Λ, thickness d, profile function $a(x)$, material refractive indices being the key ones) and on incident wave parameters (wavelength, angle of incidence, polarization). What is always very important is the connection of analysis with physical interpretation of modeling results. This also, apart from other reasons, gives legitimacy to approximate methods of grating analysis. In fact, there are two basic approaches towards the analysis, either (a) engineering approach (prediction and interpolation of a given grating behavior), and (b) physical approach (overall characterization of selected type of ODG). Both approaches will be demonstrated on examples in this contribution.

Basic ***diffraction problem electromagnetic formulation*** is schematically shown in Fig. 1, for the 1D case considered here for simplicity. The incident electromagnetic wave forms (via the interaction with a grating) sets of reflection and transmission diffraction orders.

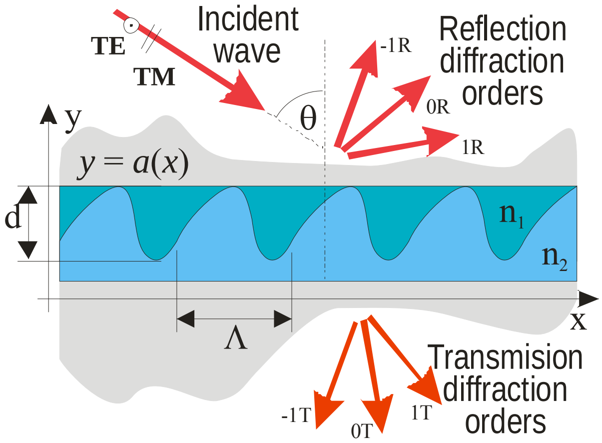


Fig. 1. Schematic picture of diffraction on a 1D relief grating.

For a complete description of the diffraction problem, both aspects of the electromagnetic field and of a grating medium must be specified, together with a choice of methodology. As to the incident field parameters, a monochromatic plane wave is often sufficient to consider, with either TE or TM input polarization, in either classical or conical mount. As to the grating parameters, for the purpose of this presentation, we will concentrate on 1D isotropic grating with a surface relief modulation, and given grating period, grating thickness, and profile function. Thus, the incident field can be considered as, e.g.

$$\vec{E}(\vec{r},t) = \exp\left[i\left(\vec{k}^{inc}\vec{r} - \omega t\right)\right],\ \vec{H}(\vec{r},t) = -\frac{1}{Z_0}\exp\left[i\left(\vec{k}^{inc}\vec{r} - \omega t\right)\right], \qquad (1)$$

where $Z_0 = \sqrt{\mu_0/\varepsilon_0}$ is the characteristic vacuum impedance.

For the TE and TM polarization, respectively, the fields will have the following vectorial components only

$$\text{TE: } \vec{E} = (0,0,E_z), \vec{H} = \left(H_x, H_y, 0\right),\ \text{TM: } \vec{E} = \left(E_x, E_y, 0\right), \vec{H} = (0,0,H_z). \qquad (2)$$

For the most typical arrangement of classical mount, the incident field vector is given by $\vec{k}^{inc} = \left(k_x, k_y, k_z\right) = \left(k_x, k_y, 0\right)$, with the magnitude of $\left|\vec{k}^{inc}\right| = k_1 = 2\pi/\lambda$. Diffractive waves in reflection and transmission orders are characterized by wave vectors $\vec{k}_m^{dif}$, for the m-*th* diffraction order.

Now, our main goal is ***to determine the distribution of energies*** (i.e. the diffraction efficiencies) ***in diffraction orders***, by solving the diffraction problem. Clearly, the solution can be considered on various levels of approximation. The basic concept of diffraction comes from the grating equation which couples together the tangential components of the wave vectors of incident and diffracted waves, for the m-*th* order, and thus determines the numbers of real propagating orders and their directions,

$$\left(\vec{k}_m^{dif} - \vec{k}^{inc} - m\vec{K}\right) \times \vec{n} = 0, \tag{3}$$

where $\vec{n}$ is the unit normal vector.

The diffraction process itself is described by the Maxwell equations or ***wave equations*** (dielectric medium, monochromatic fields) for the electric

$$\Delta\vec{E} - \mathrm{grad}\left(\vec{E} \cdot \frac{\mathrm{grad}\varepsilon}{\varepsilon}\right) + k^2 \varepsilon \vec{E} = 0, \tag{4}$$

or magnetic field

$$\Delta\vec{H} - \mathrm{rot}\vec{H} \times \frac{\mathrm{grad}\varepsilon}{\varepsilon} + k^2 \varepsilon \vec{H} = 0. \tag{5}$$

These are the starting equations for the electromagnetic analysis on a general diffraction grating. For the case of 1D gratings considered below, these equations further simplify to the two cases (TE and TM polarization, respectively), independently on z coordinate. Hence, for TE polarization, it is enough to solve the Helmholtz equation for E_z,

$$\Delta E_z + k^2 \varepsilon E_z = 0, \tag{6}$$

while for TM, for H_z,

$$\Delta H_z + k^2 \varepsilon H_z = \frac{1}{\varepsilon}\left(\frac{\partial \varepsilon}{\partial x}\frac{\partial H_z}{\partial x} - \frac{\partial \varepsilon}{\partial y}\frac{\partial H_z}{\partial y}\right), \tag{7}$$

where $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2$ is two-dimensional Laplace operator. Other field components can then be directly calculated from Maxwell equations.

To fully define the problem, ***appropriate boundary conditions*** must be next applied to the vectors $\vec{E}$ and $\vec{H}$ at all existing boundaries. For example, for a single boundary problem (surface relief boundary, given by the profile function $a(x)$, between the two homogeneous dielectric subareas 1 and 2, see Fig. 1), these will have the form

$$\vec{E}_1^{\parallel} - \vec{E}_2^{\parallel} = 0, \vec{H}_1^{\parallel} - \vec{H}_2^{\parallel} = 0, \varepsilon_1 \vec{E}_1^{\perp} - \varepsilon_2 \vec{E}_2^{\perp} = 0, \vec{H}_1^{\perp} - \vec{H}_2^{\perp} = 0, \tag{8}$$

i.e. the continuity of tangential $\vec{E}$ components and tangential and normal $\vec{H}$ components. To complete the formulation, corresponding radiation conditions must be applied to the fields found. A more detailed formulation of the diffraction problem is given in the habilitation thesis. In the following, this presentation discusses both several methods for solving such diffraction problem and usage of these methods on several modeling examples chosen. The examples presented here are based mainly on our results of Refs. 10-27.

2. METHODS OF GRATING ANALYSIS

Since the grating analysis represents quite a complicated problem, its analytic solution is possible only for some special cases and using some of the approximate approaches. This is, in fact, the case of elementary concept of diffraction on ODG based on Fourier optics (see, e.g. [3,4], also often called the ***method of complex transmittance*** or simply scalar theory of thin gratings). This approach is often used in practice, especially in such areas as classical and digital holography, even when its input assumptions are not always valid. To obtain the results in a more rigorous way, one must rely on the numerical model. Hence, traditionally, the methods of analysis are divided into approximate and rigorous ones. Clearly, there has been an ***increasing demand for rigorous approaches*** recently, due to increasing capabilities of diffractive optics technologies of complicated synthetic structures realization and simultaneously due to enlarged requests for practical applications.

Thus, ***rigorous approaches*** are based on the vector electromagnetic theory, use no assumptions, and require numerical solution. Based on a particular approach to diffraction problem, following types of methods are used: (i) ***direct numerical approaches*** (e.g. finite difference method, finite elements method, finite difference time domain method), (ii) ***application oriented approaches*** with some inherent assumptions on the character of the solution (integrated optics and photonics approaches – beam propagation methods, coupled wave methods, mode matching methods, plane wave expansion methods; diffractive approaches – boundary element method, boundary integral method; special approaches (method of fictitious and/or generalized sources); and finally ***grating approaches*** which are of primary interest in this presentation and includes modal and differential methods, based on Fourier decompositions (rigorous coupled wave analysis – RCWA, coordinate transformation method – CM), and integral methods.

On the other hand, ***approximate approaches*** are less numerically intensive (and hence also more physically transparent), but rely on series of simplifying assumptions (e.g. number of interacting waves, character of modulation, order of differential equations, etc.). Here, only the methods of interest to us are mentioned: analytic Kogelnik's coupled two wave method for volume gratings

[28], and transmittance coupled wave analysis (TCWA, [13,14]), our numerical method based on the transmittance method with coupling effects included.
In the habilitation thesis, a special attention is given to a more detailed classification and description of the methods. Also, the historical overview of the development of the analysis methods is there discussed.

2.1. Rigorous coupled wave analysis

Rigorous coupled-wave analysis, as a multi-wave second order coupled-wave theory, combines reflection and transmission behavior of a grating together. The RCWA technique belongs to such rigorous analysis methods in which the permittivity profile is expanded in a Fourier series [29]. It is based on the fact that all diffraction orders together with the evanescent waves are coupled. In this method, a single period of a surface relief grating is first divided into a large ***number of planar layers*** (see Fig. 2).

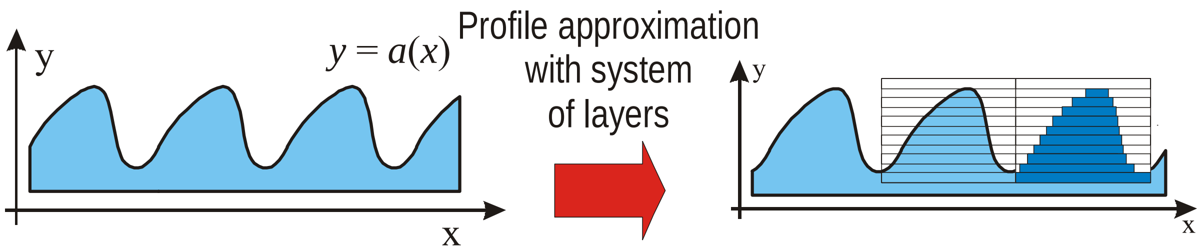


Fig. 2. Basic idea of RCWA method – approximation of a grating profile with a system of layers.

For each such a layer, the optical fields are formulated in terms of spatial harmonics using the Fourier series expansions of the dielectric constant. Effective dielectric constant of each layer is calculated as a volume-weighted average of the dielectric constants of the incident and the substrate regions. By substituting the components of these spatial harmonics into the wave equation, a sequence of coupled first order linear differential equations can be generated. The equations can be solved in terms of their eigensolutions. Next, the field distribution in each layer of the grating can be represented by the superposition of these eigensolutions. Transmission and reflection diffractive fields can then be derived by matching the appropriate boundary conditions. Subsequently, diffraction efficiencies are calculated for propagating transmitted and reflected diffraction orders. The mathematical details of the method, together with solutions of some special problems (analytical expressions for Fourier coefficients in each layer, stable algorithm for solving boundary conditions) within the efficient and stable implementation, are discussed in the habilitation thesis. Further, the energy conservation is used as a criterion for convergence of numeric solutions. The numerical effectiveness is given by the two convergence parameters, the number of orders and number of layers included in the analysis. Input parameters, namely the total number of diffraction orders, and the number of layers, are increased until the precision and the results themselves remain constant within the limits of the chosen numeric accuracy. Furthermore, to avoid numeric calculation instabilities, a modified algorithm for solving the boundary conditions have been implemented. Our RCWA model was originally used by the author mainly to model the diffraction of high spatial-frequency gratings [10], during the stay at UCSD. The implementation itself (RCWA Solver) was originally made using the Fortran language; after program debugging and testing, the solver has found its use as part of the research activities both at UCSD and home FNSPE CTU. Although only the simplest version is presented here, several further extensions and modifications have been made (lossy gratings, gratings with volume modulation of the refractive index, enforcement of the correct factorization rules for calculation with discrete Fourier expansions, TM polarization). The method has been extensively used for both physical and engineering analysis problems, and for systematic reference comparisons with approximate methods [10-18].

2.2. Coordinate transformation method

Coordinate transformation method (CM), originally developed by Chandezon, is based on the following idea. Clearly, a general curvilinear grating boundary brings in complications in solving boundary conditions [30]. In contrast to RCWA, the CM method introduces such a ***coordinate*** (non-orthogonal, curvilinear) ***transformation*** which transforms a generally complicated grating surface corrugation into a simple plane surface (see Fig. 3), hence simplifying the boundary matching problem by a great extent, but clearly simultaneously "complicating" the field equations. Next, the field equations are formulated in the new coordinates, and in analogy with RCWA, discretization by means of Floquet-Bloch theorem and Fourier expansions is performed, converting the problem into a matrix eigenvalue one. After solving this eigenvalue problem, boundary conditions are matched, fields are reconstructed, and desired diffraction efficiencies of real-propagating diffraction orders are calculated.

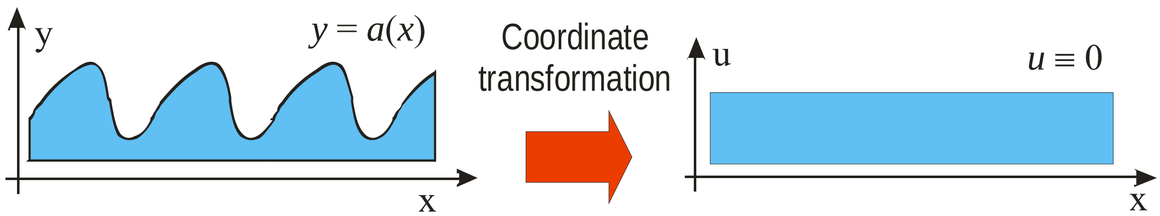


Fig. 3 Basic idea of CM method – coordinate transformation.

Our CM model, based mainly on the Li's reformulation and modification of the classical algorithm [30], has been successfully implemented and tested, and different modifications have been compared, using the computer code with a graphical interface written in the Matlab system, utilizing its possibilities (CMGraS Solver).

A comparison of the results of RCWA and CM was performed and showed a very good quantitative agreement of the simulation results. RCWA simplifies inhomogeneous grating region to the system of layers (the grating profile transforms to staircase shape), and wave equations are solved in each layer, depending on the polarization. This gives different computational demands for TE and TM polarization cases. In contrast, CM is "symmetric" with respect to the polarization with equal computational costs. Moreover, while RCWA is characterized by the two above mentioned convergence parameters, there is only one (the number of orders) in the case of CM.

We confirmed that while CM has appeared fast and efficient for smooth profiles and for both input polarizations (independently, as opposed to the RCWA), it has shown considerably slower convergence for profiles with discontinuities (e.g. multi-step profile). On the other hand, RCWA is practically ideal for gratings with multilevel profiles, it is a universal method with a stable behavior for wide range of parameters, but its efficiency (speed and accuracy) for smooth profiles is smaller. Both ***methods have been found complementary***, with a different areas of applicability in simulations, and thus both methods have been equally used in our further research, both of engineering and physical type.

2.3. Effective medium theory

The special attention has also been devoted in the last years to the approximate method of ***effective medium theory***, as the efficient tool for ***modeling of high spatial frequency*** (or subwavelength) ***gratings*** (i.e. when $\Lambda \ll \lambda$) [31,32]. Main advantages of the method are its physical transparency and efficiency. The method transfers the diffraction problem on a high spatial frequency structure to the interference problem on a homogeneous layer (or layers). In the context of subwavelength structures, we talk also about artificial anisotropy or form birefringence.

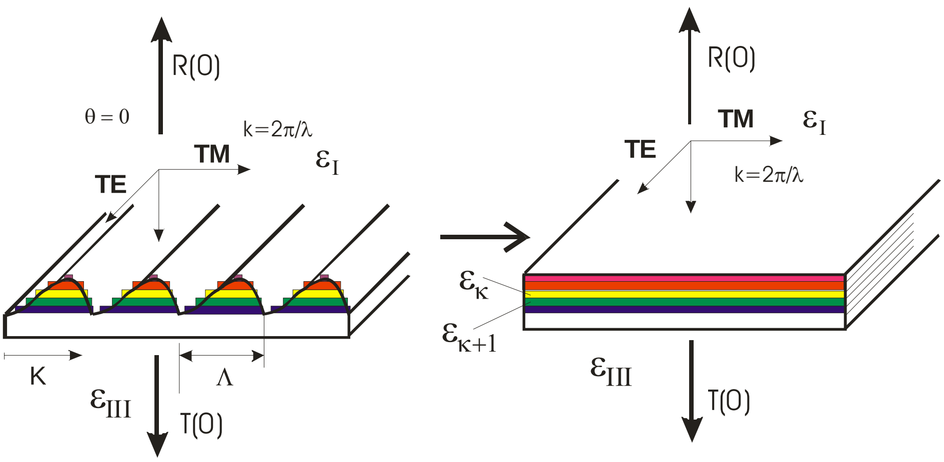


Fig. 4. Basic idea of EMT method – 1D high spatial frequency grating of a general profile and its substitution with effective homogeneous layers with effective dielectric permittivities.

Applications of subwavelength gratings cover such areas as antireflective structures, spectral and polarizing filters, splitters, and phase retarders. Concerning the physics of diffraction, the real propagating diffraction orders are here, in fact, represented only by the zero-*th* orders, all other orders are evanescent. As it appears, for the spatial frequencies far away from the first order frequency, the process of optical wave interaction with such a structure can be described through effective parameters of a medium, i.e. effective refractive indices of a homogeneous (anisotropic, uniaxial) layer, depending on the incident wave polarization).

The interaction problem is then transferred to a much simpler case of optical wave transmission / reflection on a optical layer (in the case of binary grating profile) or a system of layers (in the case of general grating profile, see Fig. 4). We have concentrated on EMT due to several reasons, in parallel and in comparison to RCWA, starting from its applications in computer generated diffractive structures and optical information processing (modeling and design of ***form birefringent microstructures*** for birefringent computer generated hologram application [33]), to development of the general modeling tool for 1D and 2D subwavelength structures [19,24].

3. MODELING OF DIFFRACTION CHARACTERISTICS

To demonstrate the models and algorithms implemented, several examples from the area of modeling diffraction characteristics will be shown, based on the results of [12,13,16-18].

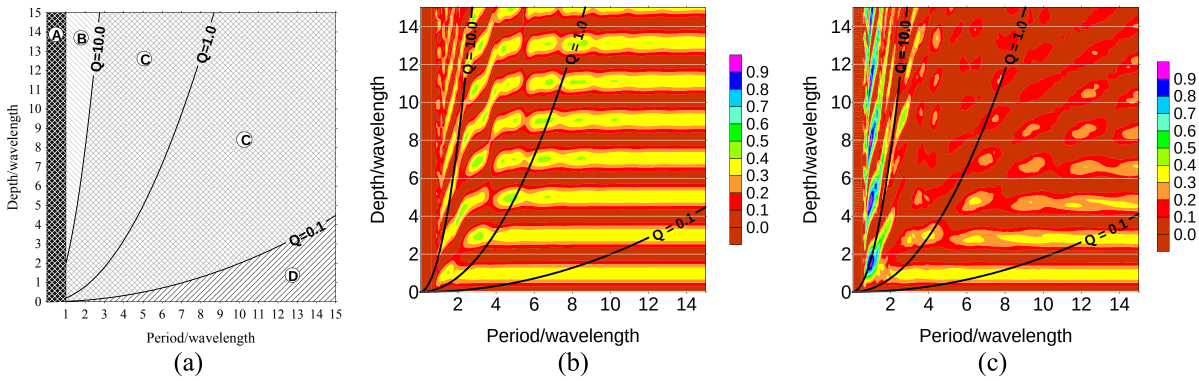


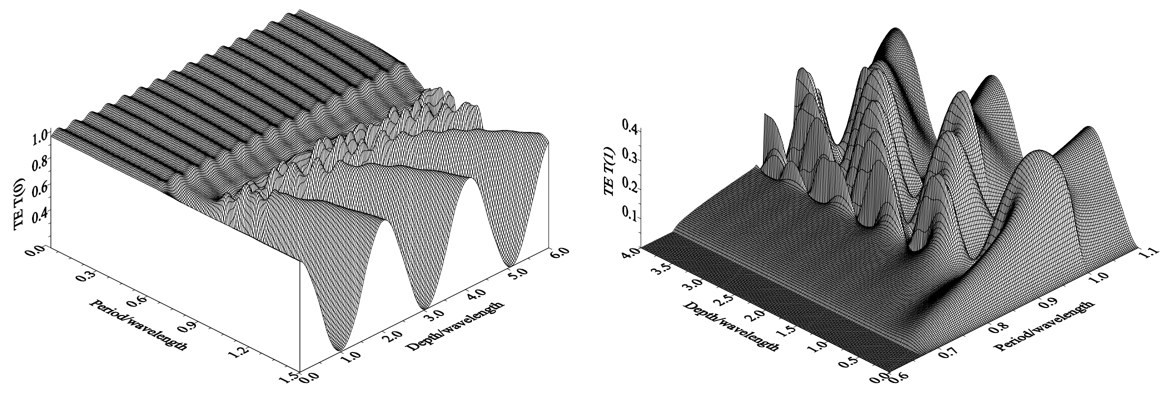
Fig. 5. (a) Schematic of characteristic regions of diffraction for a general diffraction grating, (b) example of the volume phase synchronism and characteristic diffraction regions (first diffraction order, TE polarization, grating refractive index $n = 1.5$) in $(\Lambda/\lambda, d/\lambda)$ representation, normal incidence, and (c) 30 deg incidence.

First, ***the effective representation*** of the grating diffraction efficiency has been introduced. By studying the diffraction efficiency in this representation defined by two independent variables: the period to wavelength ratio (Λ/λ) and the grating depth to wavelength ratio (d/λ) – for a fixed grating type and geometry, i.e. the angle of incidence, polarization, and particular diffraction order studied, it was possible to describe and explain the complex behavior of the grating diffraction efficiency, for the whole class of surface-relief gratings. Further, by closely looking at the whole diffraction efficiency pattern, and using the Klein volume factor [28], ***regions with typical diffraction regimes*** have been identified (high spatial frequency region, volume grating region, intermediate region, thin grating region, and resonant regions); see Fig. 5 as the example. The volume phase synchronism structure, including transversal – Fig. 5b) and Bragg – Fig. 5c) types, can also be seen in the figure. By modeling diffraction characteristics of diffraction gratings, we have contributed to better understanding and interpretation of diffraction processes and behavior in such structures.

4. EXAMPLES OF GRATING ANALYSIS APPLICATIONS

4.1. Modeling of resonant effects in gratings

Traditionally, ***grating resonances (anomalies)*** are considered as locations of sharp intense local changes (maxima, minima, oscillations) of the resulting parameters (diffraction efficiency) in parametric dependencies. Clearly, they can be both undesirable and desirable consequences for practical usage and applications [5-7]. There are basically two types of grating resonances, (1) nonresonant ***threshold*** (Rayleigh) ***resonances***, connected with the generation of new propagating diffraction orders from the evanescent ones (both transmission and/or reflection), and redistribution of diffraction orders energies; and (2) true resonant ***guided-mode resonances*** (resonances based on the induced interaction of a guided mode and interference and resonance coupling of the diffraction orders). Such guided mode resonances, due to their sharp controllable changes of diffraction efficiency (in reflection and/or transmission) with respect to key design parameters (wavelength, angle of incidence, material refractive indices) are recently having found many promising applications as ***guided-mode resonance filters*** (GMRF) [34]. In terms of the grating theory, what is responsible here is the transverse resonance, in contrast to traditional longitudinal resonance of the Bragg effect in a reflection structure. Both types of resonances have been extensively studied and modelized, with several original and interesting results [14,15,17,18].

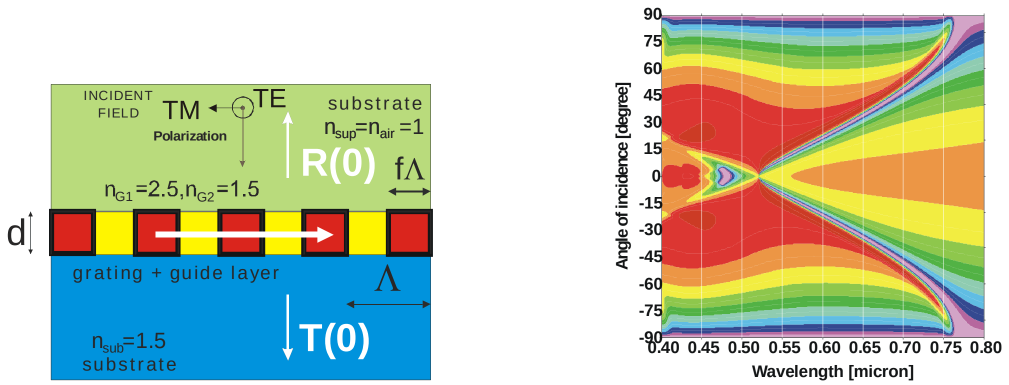


(a) (b)

Fig. 6. Example of the resonant effects modeling. Formation of the first transmission diffraction order in a binary surface-relief grating. (a) Diffraction efficiency of the zeroth T(0) order, and (b) first T(1) order. Normal incidence, grating refractive index $n = 1.5$, TE polarization.

To begin with, for example, concerning the threshold resonances, we have concentrated on the characterization of the resonant region (region E, in the $(\Lambda/\lambda, d/\lambda)$ representation). In such representation, the threshold and resonance effects are clearly separated (see Fig. 6). In this sense, we have further proposed the division of the resonant region E on the two subregions (E_1 a E_2), and we have explained and interpreted the origin of these subregions. The first part E_1, called ***the mound***, is independent on the d/λ (i.e. no volume synchronism is present here) and represents the region with an effective behavior (extension of the effective behavior of the high frequency region A). The existence conditions of this subregion have been found, depending on the relation of refractive indices of corresponding surrounding media. The second part E_2, called ***the region of resonant coupling***, has also been studied.

Concerning the guided mode resonances, we have concentrated on, e.g. the systematic ***study of various types of synchronisms*** (of e.g. zeroth reflection order); parametrical dependences on key grating and guide parameters have been studied and discussed for some typical GMRF configurations (see Fig. 7, for example).The details can be found in the habilitation thesis and in its appendices.

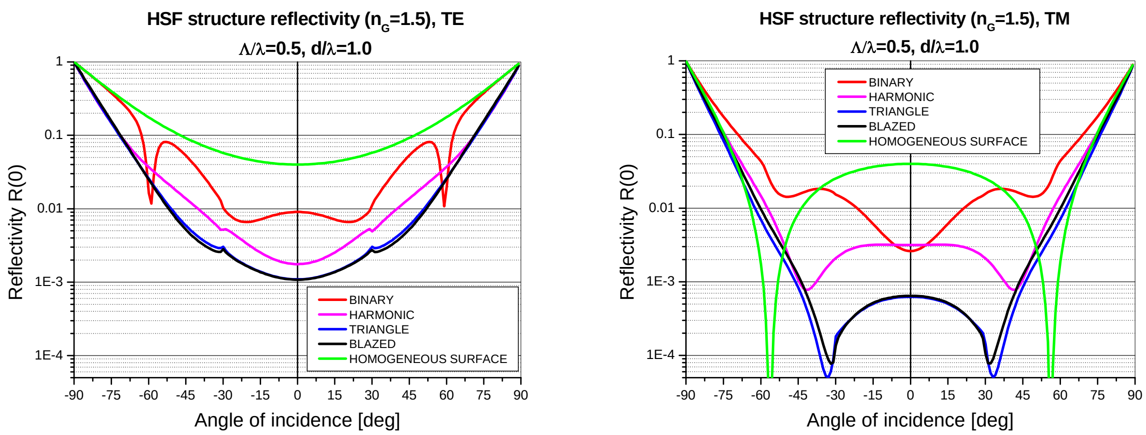


(a) (b)

Fig. 7. (a) Schematic drawing of a resonant structure – binary grating, classical mount. Material parameters chosen: grating indices n_{G1} = 2.5, n_{G2} = 1.5, index of the structure substrate n_{SUB} = 1.5, index of the structure superstrate n_{SUP} = 1. (b) Wavelength – angle of incidence synchronisms of the resonant reflectivity $R(0)$, TE, d = 0.1 µm, Λ = 0.3 µm, duty cycle = 50%.

4.2. Modeling of high spatial frequency gratings

As the second example in this presentation, modeling of ***antireflective properties*** of high spatial frequency structures will be presented. Traditionally, for antireflective properties of optical surfaces, systems of thin films are used, with their advantages and disadvantages. Another perspective alternative is newly offered with diffraction gratings with high frequency or subwavelength periods. Such structures, applying the proper diffractive optics mass production technologies, can represent effective and perspective alternative.



(a) (b)

Fig. 8. Reflectivity of microstructured high frequency grating in comparison with Fresnel reflectivities of a plane homogeneous boundary for various types of microstructure profiles (binary, blazed, triangle, and blazed profile, respectively), for TE (a) and TM (b) polarization. Relative period $\Lambda/\lambda = 0.5$, relative profile thickness $d/\lambda = 1.0$, grating medium refractive index $n = 1.5$.

From the modeling point of view, the reduction of zeroth reflection order is required. As the modeling tools, both rigorous (RCWA, CM) and approximate (EMT) methods have been used in this case. As an example, the dependencies of the reflectivities (for both polarizations) on the important design parameter – angle of incidence, are shown in Fig. 8. As can be seen, the modulation profiling is the key parameter for achievement of desired antireflective properties. For practical considerations, the applicable value of Λ/λ as well as the certain reflection homogeneity is important.

4.3. Other examples of modeling activities

Finally, due to a limited space in this presentation, other applications of modelization which have been of strong interest to us in our activities will be only briefly summarized. First of all, our ***modeling of realistic gratings*** fabricated using some of the technologies available (e.g. holographic interferometric technique, synthetic laser writer Integram, direct electron beam writer), either in our in-house laboratories, or in external cooperation (e.g. Institute of Scientific Instruments, AS CR, Brno), have consisted mainly of simulation of technological process on ideal structure deformation, i.e. modeling of fabrication inaccuracies (tolerance analysis), based on, e.g. change of profile tilt, local systematic and random profile inaccuracies, etc. Second, we have concentrated on modeling the diffraction efficiencies of ***holographically recorded sinusoidal gratings in photoresist***, the details of it being discussed in the habilitation thesis.
Next, to mention the other related activities, we have recently concentrated also on other types of structures, including (i) ***fractal diffractive structures*** and their

Fourier diffraction analysis (diffractals), (ii) ***grating couplers*** for in- and out-coupling of light from an optical waveguide [20,25], (iii) generalized periodic structures of ***photonic crystals*** (PhC) and structures based on them [21,26], (iv) modeling of ***holographic photopolymer recording media*** [22], and (v) application of direct analysis methods in ***inverse design problems*** of computer holography [27].
Concerning the recent PhC modeling activities, we have relied on our previous experience from grating analysis. Photonic crystals [37,38], from one viewpoint a generalized periodic diffractive structures, have manifested a large interest increase last years, especially due to their special properties (existence of ***photonic band gaps***) and huge application potential. Particularly, we have concentrated on mastering the basic modeling tools, ***plane wave method*** (for ideal infinite structures) and ***finite difference time domain method*** (FDTD, for both infinite – with periodic boundary conditions, and finite – with perfectly matched layer conditions), for the case of 2D structures. The work in this particular field actively continues (under the umbrella of, e.g. GACR and COST projects, especially in the area of development of the methods and their application to modelization of PhC-based structures.

5. CONCLUSIONS

The analysis of optical diffraction gratings, as the important field of diffractive and applied optics, finds many applications in both basic and applied research. The current state-of-the-art has been shown, several methods considered have been discussed, and their utilization has been demonstrated. Naturally, grating analysis methods not only save cost and time in other parts of the realization process (i.e. design, technological realization and application), but are important in basic research as well.
In the last years, several grating analysis methods, both rigorous and approximate, have been analyzed, developed, implemented, tested, and compared both to each other and to other available methods. In this presentation, the attention was given mainly to rigorous coupled wave analysis, coordinate transformation method, and effective medium theory. The methods have been applied on several levels. Within diffractive characteristics modeling activities, several new ideas concerning the classification, representation, and explicit interpretation of diffraction have been introduced. Within “application oriented” modeling activities, several problems have been approached in this presentation, e.g. resonant effects in gratings, high spatial frequency structures, realistic grating properties modeling, and structure design considerations. The methods find a wide use in many problems of diffractive and applied optics. The development of new methods of more general photonic structures analysis has also started and continued (the plane wave method, finite difference time domain method, etc.), for modeling of photonic crystal type structures. The

results demonstrate the advantages, disadvantages, and complementarity of approaches (both rigorous and approximate) studied. Simultaneously, as the various fields of optical engineering start both to specialize and, on the other hand, to link together, there will always be need for special approaches and combinations of methods.

The future research in this presented area will be concerned mainly with applications of the methods developed in practical applications within diffractive and nonlinear optics, and also with development and application of new methods (photonic crystals and microstructures, metamaterials, etc.). As already confirmed in our previous activities, the active engagement of students (mainly from physical electronics, information physics, and other specializations of physical engineering and engineering informatics) on both undergraduate and graduate levels is very valuable and beneficial, together with the direct application of research results and experience within the teaching activities.

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