Solution of the inverse problem of diffraction from low-dimensional periodically arranged nanocrystals

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ABSTRACT

The paper reports on development of an integral and nondestructive technique of characterization of low-dimensional periodically arranged nanocrystals (LDPAN) by spectroscopic scatterometry in the UV-IR ranges. Some approaches to the solution of direct and inverse problems in scatterometry are addressed. For the solution of the direct problem, the author has chosen the universal method of boundary integral equations, which has demonstrated a broad range of applicability and a high accuracy. Cases are analyzed in which a complicated three-dimensional diffraction problem involving 2D gratings can be reduced to a two-dimensional one with 1D gratings, or multilayer mirrors with plane boundaries. An algorithm is proposed for the solution of a system of nonlinear operator equations with an arbitrary, but limited set of unknown LDPAN structural parameters, and a given set of measured values of diffraction efficiency. The functional to be minimized in the course of solution of the inverse problem is identified, and methods of its regularization and for monitoring the accuracy of the solution are proposed. A Fortran code written with the use of the Löwenberg–Markwardt gradient method has turned out an efficient way to the solution of model problems for a Si grating with a trapezoidal profile.

Keywords: periodically-arranged nanocrystals, scatterometry, diffraction, inverse problem, boundary integral equations

1. INTRODUCTION

Regular ensembles of semiconductor nanowires (nanowhiskers), quantum dots (QDs), and of their combinations are arousing immense interest shared by people engaged in development of various passive and active devices for use in nano- and optoelectronics, more specifically, of light-emitting diodes, photodetectors, lasers, waveguides, and photonic crystals[1-4]. Their application produces a particular impact in such areas as photovoltaics, chemical and biological sensors, and single-photon emitters. Carrier confinement in low-dimensional nanocrystals translates into the operating wavelength becoming dependent on the size and shape of the heterostructures representing the cores of optoelectronic devices. This dictates the need of studying the morphology of ordered, nonplanar semiconducting nanomaterials and nanosystems with controllable properties. While the methods of atomic force microscopy (AFM), transmission electron microscopy, scanning electron microscopy, and near-field scanning optical microscopy are being universally used in pure research requiring analysis of the structure of nanosized objects, their application to pilot and commercial devices based on low-dimensional ordered nanocrystals meets with certain difficulties[5].

A particularly attractive probe in nondestructive and integral study of the relief and material of various nanostructures is offered by diffracted optical radiation, particularly in the x-ray, ultraviolet (UV), visible, and near-infrared (NIR) ranges. To cite an example, reflectometry and ellipsometry are employed to advantage as non-imaging optical methods to probe some structural parameters of grown LDPANs. Spectroscopic scatterometry making use of field and spectral characteristics in both reflection and transmission obtained in different configurations of the incident and diffracted radiation is capable of providing a common basis for structural analysis of LDPANs. The present author is, however, unaware of either theoretical or experimental studies made with the use of reflectometry in the near-UV, visible, or NIR ranges to probe the LDPAN structure. This paper describes the potential of a high-sensitivity metrological method based on spectroscopic scatterometry that can be applied to advantage to obtaining quantitative information on the morphology of periodically arranged LDPANs grown by molecular beam epitaxy (MBE) or any other technique, for example, by

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metal-organic chemical vapour deposition, magnetron sputtering etc.

Scatterometry is a method of optical metrology based on determination of the geometrical and physical parameters of the micro- or nanostructure under investigation (for instance, of a diffraction grating, a QD ensembles, or nanowhiskers) by measuring of the scattered field. Scatterometry includes the possibility of measuring reflected beams (reflectometry covering specular reflection) and transmitted radiation. The incident radiation must be monochromatic and can be polarized (the domain of ellipsometry). Spectroscopic scatterometry offers also the option of not only conventional angular but of wavelength λ scanning as well. The possibility of measuring and monitoring the parameters of nanosized structures, including nanocrystals, gives one grounds to assign this method to nanometrology. A brief description of the principle underlying the measurements appears to be in order here. The structure under study (a diffraction grating) is illuminated by a collimated beam of a given polarization. The intensity of the beam that became reflected from the structure or has passed through it (diffraction order efficiency), as well as the phase difference are measured as functions of λ, polarization, and angle of incidence θ of the beam (Fig. 1). The geometrical parameters and characteristics of the material of the structure under investigation are intimately related with the amplitude and phase of the diffraction orders and can be reconstructed from the measured order intensities and phase differences between the polarization components. Linear measurements by scatterometry can be performed with an accuracy of to within a few fractions of a nanometer or even better, which is hundreds of times smaller than λ employed in the measurements. Scatterometric equipment employed in experiments includes ellipsometers or monochromators combined with goniometers. The set of diffraction order efficiencies and phase differences measured for preset parameters of the incident radiation is usually referred to as the signature. On completion of the measurements, determination of the parameters of the diffraction grating reduces to solving the inverse problem, which consists essentially of reconstruction of the geometric or material parameters (optical constants) of the structure from the measured signature. Solution of the inverse problem requires as a necessary prerequisite solution of the direct problem of diffraction of a light wave from a grating with known boundary parameters and optical constants, which should be obtained by one of the rigorous methods of diffraction theory.

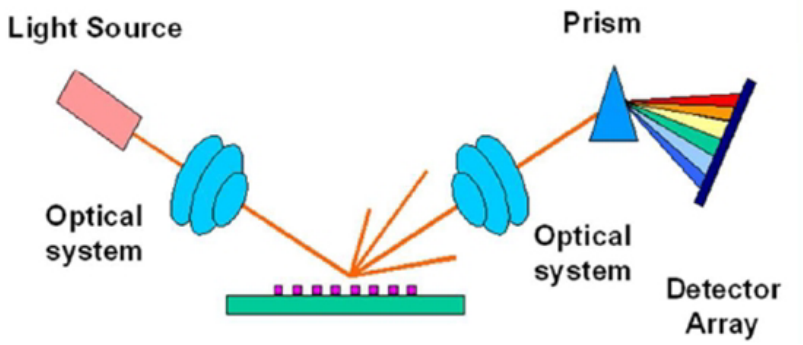

Figure 1. Schematic of a spectroscopic scatterometry setup.

We have developed an appropriate software package PCGrate®[6] (Fig. 2) based essentially on the modified method of boundary integral equations[7-10] (MIM), which was developed for solution of such direct diffraction problems. The PCGrate provides, in particular, solution of diffraction problems involving multilayer gratings, photonic crystals, and multilayer coatings. The convergence rate, accuracy, reliability, and versatility of such software may cut by 90% the difficulties involved in solution of extremely ill-conditioned, time and memory consuming inverse scattering problems. The PCGrate was successfully used to solve a variety of inverse scattering problems, among them determination of the refractive index in the vacuum UV range of thin MgF_2 films which were deposited on the surface of a multilayer diffraction grating with a real (AFM measured) groove profile[8]; determination of the heights and side-wall slopes in MBE-grown single and multilayer QD ensembles in In(Ga)As/GaAs and Ge/Si systems from analysis of specular and diffuse x-ray scattering[5,11]; and deriving the NIR refractive indices of thin ZrO_2 films from given absorption in the ZrO_2/W system with heteroboundaries of different geometries[12]. The PCCgrate code is composed in the C++ language, but the author has at his disposal its earlier Fortran version. Modified by introducing some changes and complements, including, in particular, the possibility of reducing the problem of diffraction from bi-periodic (2D) gratings to that from one-periodic (1D) ones, it is employed as a part of the software package designed for solution of the inverse problem in LDPAN scatterometry in the context of the present work. Sections 2 and 3 deal with some techniques used in solution of direct scattering problems.

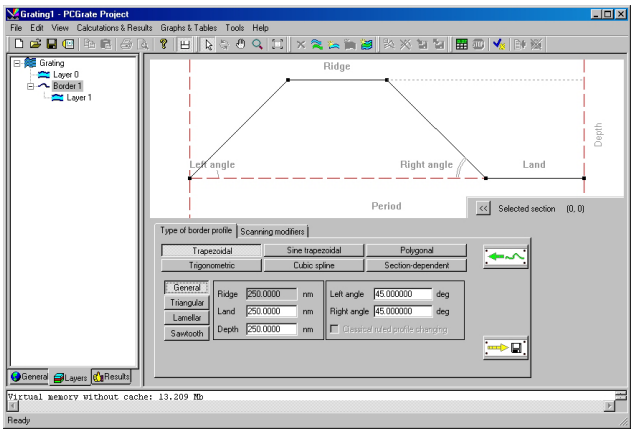

Figure 2. General trapezoidal profile obtained by cutting the surface of a grating with one vertical plane.

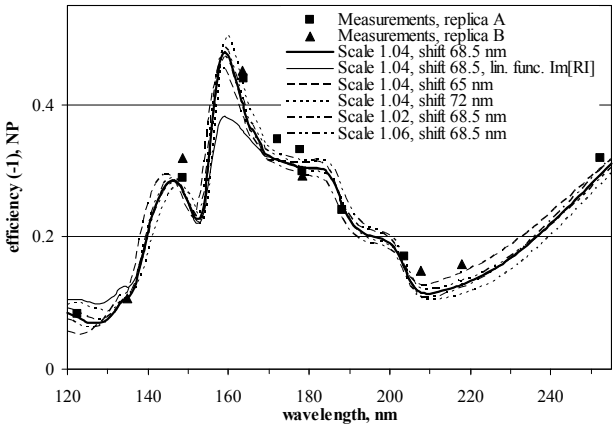

Figure 3. Measured (symbols) and calculated (curves) non-polarized efficiencies of G185M grating plotted vs. λ.

Several were proposed for solution of the inverse scatterometry problem; they involve methods were proposed for solution reconstruction of the geometric or material parameters of a structure from the measured signature. In a general case, these methods are generally aimed at solution of a system of nonlinear operator equations, subject to some initial conditions and capable of providing the desired accuracy, because both the measured quantities and those derived from the direct method are known to within an error. The efficiency of any optimization algorithm depends on the condition of the goal function chosen, which is usually found from the difference between the corresponding measured and calculated signatures. All methods developed for solution of the inverse problem can be classed among several types, namely, global, local, mixed etc. In the present work, the solution of the inverse scattering problem is based on the Löwenberg-Markwardt algorithm, which is essentially an optimization approach aimed at solution of least-squares problems and is stable against errors in the initial data and their small number. The proposed algorithm is actually a modified Gauss-Newton method, which has demonstrated its potential in dealing with inverse problems in scatterometry of nanosized structures[13,14]. The approach used in the solution of inverse scattering problems is discussed at length in Sections 4 and 5. Section 6 highlights the results of a trial numerical experiment in a particular example of a model grating with an equal-sided trapezoidal profile in the perpendicular section.

2. METHODS OF SOLUTION OF THE DIRECT PROBLEM FOR A PERIODIC DIFFRACTION STRUCTURE

Numerical methods are ordinarily employed in treating diffracting structures whose characteristic dimensions, more specifically, period d, diffraction zone width, correlation length, depth h, etc) are comparable with the wavelength of the incident radiation ($\lambda / d \sim 1$), i.e., in the resonance region. Structures with subwavelength dimensions require solution of the direct problem in terms of electromagnetic theory, in other words, of Maxwell's equations with rigorous boundary conditions and radiation conditions. Theory offers presently rigorous numerical methods to solve problems of diffraction from multilayer (multiboundary) 1D and 2D gratings with arbitrary groove profiles, which can conveniently be assigned to two branches, integral or differential, of electromagnetic theory. The first of them includes, again by convention only, methods involving finite elements (including boundary and volume), fictitious sources, and integral equations (boundary and volume). Some methods resembling closely the differential approach, among them the modal (referred to sometimes as characteristic-wave or characteristic-modal) method, coupled-wave (Fourier-modal) method, and method of coordinate transformation are classed by some researchers among a special group[15,16]. They all are based essentially on Maxwell's equations in partial derivatives. In a general case, differential theory includes typically integration of these equations over one or two coordinates. Most of the currently used differential methods resort to one-dimensional integration or some other numerical approach in solving a system of conventional differential equations. The method of boundary integral equations treats Maxwell's equations in the integro-differential form, with their subsequent numerical solution by curvilinear integration. Some versions of the finite-element method can also be assigned to the integral theory[17]. In contrast to the method of integral equations, this approach assumes, as a rule, two-dimensional integration, the only exclusion being the method of boundary integral elements. Drawing basically close to the method of integral

equations is that of fictitious sources[18]. For a comprehensive review of a large number of theoretical treatments and their mathematical realizations, the Reader is referred to the abovementioned publications and references therein.

An approach most frequently followed when considering scattering from ordered objects, including scatterometry and, particularly, 2D gratings, is the straightforward and readily tractable rigorous coupled-wave analysis (RCAW), called also customarily the method of Moharam and Gaylord[16]. We are going to dwell on it in some detail to be able to compare its advantages and shortcomings with the method of boundary integral equations employed by the present author in treating the direct problem. In many problems of diffraction monochromatic light is used. Analysis of these problems requires solution of the Helmholtz equation (in its wave form). If we restrict ourselves to consideration of periodic objects only, for example, to 1D or 2D diffraction gratings, and 2D or 3D photonic crystals, this method will turn out particularly appropriate for operation with the Helmholtz equation. The first to apply it, albeit not in a rigorous formulation, to analysis of volume holograms was Kogelnik in as far back as 1969. M. Moharam and T. Gaylord applied the coupled wave method to analysis of diffraction gratings in its rigorous formulation, at any rate, for gratings with lamellar (rectangular) profile in 1981[19]. The RCWA treats the electromagnetic field in homogeneous regions of space, in front of a periodic object and behind it, as comprised of a linear combination of plane waves. For a nonperiodic confined object one has to accept, in place of a linear combination of plane waves, a continuous expansion in plane waves in the form of the Fourier integral. In the region of the object, Maxwell' equations are solved by Fourier transformation. To find the unknown coefficients in the Fourier expansions, a system of linear algebraic equations is formulated. Application of the RCAW to classical (2D) diffraction problems with one-periodic boundaries, i.e., with a stepwise changing dielectric and/or magnetic permeability at the boundary is essentially different for the TE and TM cases (with the electric vector confined to the plane perpendicular to the plane of the wave vector **k** and parallel to the grating grooves, or lying in the **k** plane, respectively). In the case of the TE polarization, the unknown electromagnetic field $u(x, y)$ field and its normal derivative remain continuous at the boundary. For the TM polarization, the normal derivative suffers a discontinuity, which is responsible for all subsequent problems associated with convergence and accuracy of the method, a factor that nobody has yet found a way to combat. While the RCAW intuitively appears to be tractable, the present author is unaware of any mathematical publications which would offer a rigorous substantiation of its convergence, even for a smooth $|\mathbf{k}| = k(x, y)$ relation. The main difficulty standing in the way of such a substantiation is the exponential growth of the elements of transmission matrices[16] along the rows and columns. This growth gives rise to numerical problems; matrices and the corresponding systems of differential equations are poorly conditioned; indeed, their eigenvalues belong to different scales, and this effect is the stronger, the more harmonics are taken into account[20]. Obviously enough, diffraction problems with a discontinuity of k at the interfaces will meet with the natural constraint on the convergence rate for the RCAW. Indeed, the Fourier coefficients of $k^2(x, y)$ and $u(x, y)$ cannot approach zero fast enough for the y = const line which crosses the boundary. The best version of factorization available thus far for the RCAW and other similar methods of the differential group in the TM polarization[16] called Fast Fourier Factorization, enjoys presently wide recognition. Its authors have, however, revealed the remaining abovementioned limitations of a fundamental nature which place a constraint on the use of this approach in cases of high conductivity in the TM polarization[21]. Besides, application of the RCAW to non-lamellar profiled gratings involves discretization into plane layers, the so-called staircase approximation. This approximation was shown[22] not to be rigorous; indeed as the number of the layers increases, the result obtained in solution of the equations will not necessarily tend to accurate values. In the case of the TE polarization and 1D gratings, the convergence of this approximation is, as a rule, good, but in the TM case an increase in the number of layers does not improve the results; on the contrary, they begin to diverge. This can also be seen from an analysis of the properties of the solution in the case of one layer and the TM polarization[23]. The conclusions drawn for the case of 2D diffraction from 1D gratings with one boundary will naturally hold for multilayer gratings, conical (3D) diffraction and bi-periodic gratings. Nevertheless, for lack of a better alternative, the RCAW is widely used for 1D and 2D gratings in micro-optics analysis and waveguide technology, as well as in problems involving synthesis, for instance, of multi-order diffraction gratings or diffraction elements with preset characteristics[24].

The method of boundary integral equations is presently universally recognized as one of the most developed and flexible approaches to an accurate numerical solution of diffraction grating problems (cf. Refs.[25-27] and references therein). Viewed in the historical context, this method was the first to offer a solution to vector problems of light diffraction by optical gratings with a high enough accuracy and to demonstrate remarkable agreement with experimental data[6]. This should be attributed to the high accuracy and good convergence of the method, especially for the TM polarization plane[26,28]. It does not involve limitations similar to those characteristic of the RCAW, and it provides a better convergence. To disadvantages of this method belong its being mathematically complicated, as well as numerous "peculiarities" involved in numerical realization. Besides, application of the integral method to cases of heterogeneous or

anisotropic media meets with difficulties. Nevertheless, it is on the basis of this theory that all the well-known problems of diffraction by the periodic and non-periodic structures in optics and other fields have been solved. In many cases it offers the only possible way to follow in research[15,29,30]. The flexibility and universality inherent in the integral method, in particular, enable one rather easily to reduce the problem of radiation of Gaussian waves or of a localized source to that of plane wave incidence, for which scientists all over the world have a set of numerical solutions. Generalizations of the integral method have been recently proposed for arbitrarily profiled 1D multilayer gratings[31]; randomly rough x-ray–extreme-UV mirrors[9]; conical diffraction mounts[28]; and arbitrarily rough multilayer 1D gratings and mirrors[10].

This part of the paper will highlight, necessarily briefly, only the fundamentals of the MIM employed by us, and point out some of the advantages it offers in analysis of LDPANs compared with other available numerical approaches. The author will also discuss the possibilities particularly appropriate for LDPANs, namely, those of reducing the problem of diffraction from bi-periodic surfaces of a given symmetry to an equivalent problem applicable to 1D gratings or multilayer structures with plane boundaries. Details of the method and of its numerical realization for 1D gratings were covered in the literature cited above, and the theory for 2D gratings will be published elsewhere. The rigorous formulation of the problem of diffraction from 2D gratings with a finite conductivity of their material and an analysis of the existence, uniqueness, and stability of the solution, as well as some close approaches to finding this solution drawing from variation methods and integral equations can be found in[25,32,33]. It is known that for all but possibly a discrete set of frequencies the direct scattering problem has a unique weak solution in the case of bi-periodic inhomogeneous media in the whole $\mathbb{R}^3$, of which an absorbing medium always leads to uniqueness result for any frequency.

The electromagnetic formulation of diffraction by gratings, which are modeled as infinite bi-periodic structures, can be reduced to a system of Helmholtz equations for the vector components of the electric and magnetic fields in $\mathbb{R}^3$, where the solutions have to be quasiperiodic in the x- and z-directions, subject to radiation conditions in the y-direction, and satisfy certain boundary conditions at the interfaces between different materials of the diffraction grating. The integral method is an approach which allows us to reduce in a rigorous manner a problem of diffraction by a grating (i.e. respective Helmholtz equations) to solving a linear boundary integral equation or a system of such equations. In general, the integral approach, as well as the similar finite-element method, involves two-dimensional integration. However, in actual practice, a one-dimensional curvilinear integration easily reduced to ordinary integrals is used. The Green's theorem and boundary integral (potential) operators, i.e. a combination of the direct and indirect approaches, are applied here as described in[25,34]. Then the linear integral equations so obtained are reduced to a system of linear algebraic equations by the collocation method or by the Galerkin method. In practice, the convergence and accuracy of efficiency computation depend significantly on a proper choice of trial functions, discretization schemes, and respective quadrature rules. In our realization, we use a rather simple but robust, universal, and fully discrete technique, the so-called classical Nyström collocation method[26]. The process of numerical solution of integral equations is based on collocation with piecewise constant or trigonometric plus cubic spline test functions[9,28]. The principal parameter, by which the convergence is estimated, is the number N of collocation points at each boundary. The collocation points and the quadrature nodes can be chosen independently of one another or selected at the same locations. The latter choice (in our programs, it is option by default in most cases) requires standard regularization of integrals. It is worth noting that the regularization is used even at corner nodes of a non-smooth boundary. For relatively shallow profiles, the nodes can be uniformly arranged along the x- and z-coordinates (grating periodicity)[30]. But a uniform distribution with respect to the arc length, as shown in[7,29,35] is more universal and makes it possible to treat in boundary cross sections, for example, severely asymmetrical, non-functional as lamellar, or even closed profiles by the integral method, without any additional effort at the user's end. In a narrow sense, the MIM is a collocation method which also specifies a direct summation rule for Green's functions and their derivatives (Green's series). In the simplest case, the corresponding series is truncated symmetrically at the lower summation index $-P$ and the upper index $+P$, where P is an integer defined by $P \approx \kappa N$. The "truncation ratio" κ is optimized at small values of N and is kept constant as N increases. It has been found[7] that $\kappa = 0.5$ is a reasonably good option for most practical calculations. Quadratures in our codes are performed by the rectangular rule with the following single-term corrections: for Green's functions, we take into account its logarithmic singularity; for normal derivatives of Green's functions, we allow for the profile curvature, and for tangential derivatives, we take into account the non-integrable singularity. For gratings with smooth boundaries, this method yields an overall error estimate $O(N^{-3})$ for the diffraction amplitudes and efficiencies in both polarization planes. However, the above simple truncation rule for Green's series is inadequate to match such accuracy of the collocation. An efficient remedy is provided by Aitken's acceleration procedure[36] applied to the truncated Green's series. Instead of the direct summation algorithm used in the MIM, more sophisticated methods can be implemented to accelerate the computation of integral kernels for conical diffraction problems[28].

3. REDUCING THE PROBLEM OF DIFFRACTION FROM A 2D GRATING TO THAT FROM 1D GRATINGS OR A MULTILAYER MIRROR

The large complexity of the solution of inverse problems of scattering from bi-periodic multilayer structures of a general kind confers particular significance to the possibility of reducing these difficulties to a simpler approach, for instance, to an analysis of 2D diffraction from 1D gratings or a multilayer mirror. This reduction is of particular significance for express and *in situ* diagnostics. It can be effected for some angular relation between the incident radiation and the diffraction structure, for example, in the case of normal incidence onto the horizontal plane of a grating structure (x, z) with equal periods and some symmetric boundary function. Such a case is typical of many LDPANs; therefore, in this part the author is going to discuss at some length the possibilities available for this purpose.

Equivalent rules for determination of the efficiencies of reflected orders of 2D gratings from those calculated for 1D gratings can be found in[25]. The approach used is based on expansion of the efficiency of a bi-grating with profile boundaries symmetric relative to the horizontal plane in a Taylor series in powers of h, with the principal terms of the series retained in the $h < d$ case. Then the efficiencies $e_{0,m}^{+}$ and $e_{0,n}^{+}$ (see Section 4) of the orders numbered (0, m) and (n, 0) propagating in the upper (+) medium for arbitrary linear polarization of light can be defined through the leading (quadratic in h) terms of the expansion as

$$e_{0,m}^{+} = e_{0,1}^{+} e_{m,2}^{+} / R;\ e_{n,0}^{+} = e_{n,1}^{+} e_{0,2}^{+} / R, \tag{3.1}$$

where $e_{n(m),1(2)}^{+}$ are the values of the efficiencies of the corresponding mutually perpendicular 1D gratings calculated with the position of the polarization vector left unchanged, and R is the Fresnel reflection coefficient of the grating material. As follows from a comparison with the results of rigorous calculations performed in[25] and by the present author, the approximate relations (3.1) give a high-accuracy solution for two cases: (1) $h << d\ \Lambda\ \lambda < d$, and (2) $h <$ d $\Lambda\ \lambda > d$. The results obtained in such a comparison will be published elsewhere. Close to the Rayleigh wavelengths (appearance of orders), the accuracy of the method becomes notably worse. In the cases where the real part of the refractive index of the grating material is small, the profile depth h can be large enough, even larger than d, which has particular significance for the field of application. In both cases, low efficiencies of the first (principal) diffraction orders may be considered as a criterion of converging results of the approximation (3.1).

Another simple method applicable to determination of the efficiency of bi-periodic gratings is the effective medium approximation (EMA) developed for such structures in Ref.[37]. For $\lambda >> d$, a wave does not respond to the structure of the relief, and the intensity of reflection (only the 0th reflection order exists in these conditions) is determined only by the effective refractive index, which is different for different polarizations. Now the bi-periodic grating structure is replaced, in a general case, with a plane-boundary multilayer structure (a multilayer mirror), whose reflection/transmission coefficients can be calculated in a very short time and with any desired accuracy with the use, for instance, of the S-matrix approach[38]. The effective refractive index $n_{2D}^{(0)}$ of a medium filled by a 2D grating can be calculated in the zeroth order of the EMA using the following relations

$$\begin{aligned} n_{2D}^{(0)} &= [n' + 2\tilde{n}_{2D}^{(0)} + 2n''_{2D}{}^{(0)}] / 5,\ \ n' = (1-f^2)n_1 + f^2 n_2,\ \tilde{n}_{2D}^{(0)} = [(1-f)\varepsilon_1 + f\varepsilon_p^{(0)})]^{0.5}, \\ n''_{2D}{}^{(0)} &= [(1-f)/\varepsilon_1 + f/\varepsilon_s^{(0)}]^{-0.5},\quad \varepsilon_s^{(0)} = (1-f)\varepsilon_1 + f\varepsilon_2,\ 1/\varepsilon_p^{(0)} = (1-f)/\varepsilon_1 + f/\varepsilon_2, \end{aligned} \tag{3.2}$$

where f is the filling factor, ε_1 and n_1 are the dielectric permittivity and the refractive index of the medium separating the LDPANs ($\varepsilon = n^2$), ε_2 and n_2 are those of the LDPANs, ε_s (TE) and ε_p (TM) are the parallel and perpendicular polarization components of the dielectric permittivity. It is known that the EMA is a good approximation not only for $\lambda >> d$ but for $\lambda \sim d$ as well, provided $|\varepsilon_2 - \varepsilon_1|$ is not too large, and one uses the second-order EMA, which allows for the λ / d ratio[37]. An analysis performed by the present author suggests that, for instance, for $\varepsilon_1 = 1$, $\varepsilon_2 = 9$, dielectric permittivity of the substrate $\varepsilon_{sub} = 9$ and a small filling factor f, the orders propagating in the substrate do not practically affect the 0th reflection within a large range of the λ / d ratio and angles of incidence for any polarization of the incident radiation. The imaginary part of the LDPAN refractive index likewise affects only weakly the convergence of the results of calculations, particularly in the TE polarization. Significantly, a grating with a more complicated (non-lamellar) groove profile may be considered as a multilayer mirror by discretization of the profile into several regions which are homogeneous in the vertical direction[39]. Said otherwise, the second-order EMA broadens the range of applicability of equivalent rules to high-frequency gratings, so that when combined with the above rules of analysis of a 2D grating as combinations of 1D gratings it extends to cover a large number of LDPAN cases. The other cases, just as checking the applicability of various approximations, should be analyzed by rigorous solution of the direct 3D diffraction problem with 2D gratings by methods employed in scatterometry.

4. METHODS OF SOLUTION OF THE INVERSE PROBLEM IN SCATTEROMETRY

Irrespective of what rigorous method of analysis was employed, the inverse scattering problem can be solved by an optimization technique. The criterion that should be optimized (or minimized), is the rms deviation of the calculated diffraction order intensities from the measured (preset) values. Solution of the inverse problem in scatterometry consists essentially in reconstructing the geometric or material parameters of a structure from the measured signatures. The efficiency $e_{k,l}^{\pm}$ of the orders propagating in both media (the lower medium is labeled by "–") is defined as

$$e_{k,l}^{\pm} = |A_{k,l}^{\pm}|^2 \beta_{k,l}^{\pm} / (\beta c^{\pm}), \tag{4.1}$$

where $A_{k,l}^{\pm}$ are the amplitudes of the (k, l)-th propagating harmonic of field expansion in a Fourier series for the TE polarization (see Section 5), β and $\beta_{k,l}^{\pm}$ are the y-components of the incident and diffraction wave vectors, and $c^{+} = 1$ for the upper half-space, and $c^{-} = \tau$ for the lower half-space ($\tau^{-1} = \mu^{+} / \mu^{-}$ for the TE polarization, and $\tau^{-1} = \varepsilon^{+} / \varepsilon^{-}$ for the TM). The phase difference can be written as

$$\arg[A_{k,l}^{\pm} / |A_{k,l}^{\pm}|] - \arg[B_{k,l}^{\pm} / |B_{k,l}^{\pm}|], \tag{4.2}$$

where $B_{k,l}^{\pm}$ are the amplitudes of the (k, l)-th propagating harmonic of Fourier expansion of the field for TM polarization.

The sets of data measured at given angles of incidence, wavelengths, and polarization states, or a part of these data sets have to be used to derive the periodic grating corresponding to these data. Unfortunately, from the mathematical standpoint this problem is essentially ill-posed. Development of a general theory of the existence of a solution and of its uniqueness for such problems is still not complete, and analyses of some particular cases are far from being trivial[40-42]. The uniqueness issue is always important in looking for efficient reconstruction algorithms in practical applications. Experimental errors, no matter how small, entail huge errors in reconstruction of the profile of a grating structure. While the regularization techniques employed improve noticeably solution of ill-conditioned problems[21], their accuracy is substantially lower than that of solution of the corresponding well-conditioned problems. One can improve reconstruction by using a large number of a priori reliable data. This can be reached, for instance, by restricting the search to simple types of possible gratings defined by several parameters. In this way an ill-conditioned problem can be reduced to a well-conditioned parametric reconstruction.

We are turning now to gratings of a fixed type described by a parameter vector $\mathbf{p} = (h_n)$, $n \in N$ of material parameters h_n and a natural index n. These parameters may include geometric parameters and refractive indices. The LDPANs are assumed to be arranged on a 2D square grid with identical profiles of trapezoidal boundaries (Fig. 2) in two perpendicular cross sections. We assume also that the efficiencies and phase differences respond slowly to a small variation of these grating parameters. We assume, as done in[13], that the set of allowable (physically realizable) parameters is limited by their upper and lower boundaries:

$$h_n^{\text{low}} \le h_n \le h_n^{\text{up}},\ n \in N \tag{4.3}$$

Let us now determine the signatures of the measured efficiencies and phase differences which form the data base for the grating reconstruction, with the use of the relation (E_m), $m \in M_0$. To be more specific, for each $\mathbf{p} = (h_n)$, $n \in N$ set there is a corresponding set of the values of efficiencies and phase differences $(E_m(\mathbf{p}))$, $m \in M_0$. We define the measured values corresponding to the exact solution to be reconstructed by $(E_m^{ex}(\mathbf{p}))$, $m \in M_0$. Hence, the inverse problem consists in determination of an optimum set of parameters $\mathbf{p}^{\text{op}} = (h_n^{\text{op}})$, $n \in N$, which satisfy (4.3) and are such that

$$(E_m(\mathbf{p}^{\text{op}})) = (E_m^{ex}),\ m \in M_0. \tag{4.4}$$

Measured values are not exact; therefore, the existence of solution (4.4) is not certain. Introduce an error function $f(\mathbf{p})$ which depends on the grating parameters (vector $\mathbf{p}$) and the difference between the measured signature and the signature for the $\mathbf{p}$ parameters. All the available methods involve minimization of this error function. And it is vector $\mathbf{p}$ providing the minimum that is the estimate of the parameters. This set of the optimum parameters is derived usually by minimizing the sum of the squares of the differences between the measures values of the scattering intensity which characterize the object, and the corresponding values obtained from the solution of the direct diffraction problem. In this case, we are looking for the parameter vector $\mathbf{p}^{\text{op}} = (h_n^{\text{op}})$, $n \in N$ which satisfies Eq. (4.3) and is such that

$$\begin{aligned} f(\mathbf{p}^{\text{op}}) &= \min f(\mathbf{p}),\ \mathbf{p} = (h_n),\ n \in N; \\ f(\mathbf{p}) &:= {}_m\Sigma |\, E_m(\mathbf{p}) - E_m^{ex}|^2,\ m \in M_0. \end{aligned} \tag{4.5}$$

There are different well developed optimization approaches applicable to Eq. (4.5), among them best fit, global stochastic algorithms, gradient local methods, neural network methods, and various hybrid techniques, for example[43-45]. It is known that local methods provide, by and large, a locally optimal solution. The question of which from among several available methods to choose rests upon many factors, for instance, the complexity of the direct problem, the available computing storage capacities, the time reserved for solution of the inverse problem, the required accuracy of the solution, the experimental data base amassed, and the extent to which the properties of the solution of the direct problem match the optimization approach chosen. With a correctly chosen approach, a simple optimization method may be found appropriate. To cite an example, a least-squares procedure combined with straightforward fitting were found adequate in determination of refractive indices of a thin protective non-conformal MgF_2 layer with complicated AFM-measured boundary profiles developed for the UV multilayer flight gratings installed on the last servicing mission to the Hubble space telescope[8] (Fig. 3).

Let us dwell, necessarily briefly, on the fundamentals of any optimization approach. Details of the Löwenberg–Markwardt gradient method chosen for solution of the inverse scattering problem will be described in Section 5. Other methods are discussed in considerable detail in the literature cited above. Consider the inverse problem in a simple example of reconstruction of a trapezoidal-profiled 1D grating (Fig. 2) which was subsequently used in testing of the algorithms developed. The profile of an LDPAN arranged on a grid with a nanowhisker growth cone, or of a QD of a pyramidal shape can be described in cross section in the simplest case with an equal-sided trapezoid. This profile is uniquely defined by **p** with $N = 3$, namely, length of the base $b = d - Land$, h (*Depth*), and the angle between the side and the height α (*Left angle = Right angle*). Assuming d and the refractive indices of the grating and substrate materials to remain unchanged, determination of the grating profile parameters reduces actually to finding three parameters (h, b, α) from the signature with the use of Eq. (4.5). Thus, any signature depends not only on the parameters of an incident plane wave (angle, polarization, wavelengths) but, in its turn, on h, b, α of the diffraction grating. The length of the signature (the number M_0 of measurements) depends on the parameters of the problem and methods of its solution and is chosen based on other considerations. In a numerical procedure, it appears more appropriate to reconstruct not the angles but rather the relative coordinates of some vertices of the boundaries of the structure under consideration, which promises a richer choice of options. In the particular example of a symmetric trapezoid there are five such vertices, with only three of them being independent. Next one calculates the signature for different wavelengths, incidence angles, and polarization states. The method proposed permits one to derive from the condition of minimization of the goal function (see Section 5) estimates of the parameters, which are to be compared with the starting figures. A comparison of the parameters found in some way with the estimates obtained yields finally the accuracy of calculation of the parameters.

5. LÖWENBERG–MARKWARDT OPTIMIZATION ALGORITHM

As already mentioned, inverse problems of the type considered here belong to the class of ill-posed problems. The reasons for this could be traced to the insufficient setmof the measured data available, errors in measurements and calculations, and inadequate mathematical description of the object being modeled. Methods proposed for solution of ill-conditioned problems are based on the concept of a regularizing algorithm which is resistant to errors in the starting data. This Section will deal with the Löwenberg–Markwardt (LM) optimization algorithm[43] developed for inadequately informative signatures and describes its regularizing properties conducive to efficient operation. The efficiency of an optimization algorithm depends strongly on the extent to which the goal function is conditioned. A local goal function can be written as

$$f(\mathbf{p}) \approx \|(E_m(\mathbf{p}^{\mathrm{ex}})) + A^{\mathrm{ex}}{}_{M0N}(\mathbf{p} - \mathbf{p}^{\mathrm{ex}}) - (E_m{}^{ex})\|^2;$$
$$A^{\mathrm{ex}}{}_{M0N} := (\partial E_m(\mathbf{p}^{\mathrm{ex}}) / \partial p_n),\ m \in M_0,\ n \in N, \tag{5.1}$$

where the gradient of this approximate functional is $2\mathbf{p}[A^{\mathrm{ex}}{}_{M0N}]^{\mathrm{T}}A^{\mathrm{ex}}{}_{M0N}$ + constant. Neglecting some constraints, minimization of a quadratic functional is equivalent to solving a matrix equation with the $[A^{\mathrm{ex}}{}_{M0N}]^{\mathrm{T}}A^{\mathrm{ex}}{}_{M0N}$ matrix. Hence, the condition number $\mathrm{cond}([A^{\mathrm{ex}}{}_{M0N}]^{\mathrm{T}}A^{\mathrm{ex}}{}_{M0N})$ defines the condition of f.

An alternative to optimization of f by the method defined by Eq. (4.5) is application of the LM method directly to Eq. (4.4)[13]. Similar to Eq. (5.1), we can write

$$(E_m{}^{ex}) = (E_m(\mathbf{p}^{ex})) \approx E_m(\mathbf{p}) + A_{M0N}(\mathbf{p}^{ex} - \mathbf{p}),\ m \in M_0;$$
$$A_{M0N} := (\partial E_m(\mathbf{p}) / \partial p_n),\ m \in M_0,\ n \in N;$$
$$A_{M0N}(\mathbf{p}^{ex} - \mathbf{p}) \approx (E_m(\mathbf{p}^{ex})) - E_m(\mathbf{p}),\ m \in M_0. \tag{5.2}$$

Solution by the least-squares method of the non-quadratic linear system (5.2) can be written as

$$\mathbf{p}^{ex} = \mathbf{p} + [[A_{M0N}]^{\mathrm{T}} A_{M0N} + \mu E]^{-1} [A_{M0N}]^{\mathrm{T}} [(E_m{}^{ex}) - (E_m(\mathbf{p}))], \tag{5.3}$$

where μ is the regularizing coefficient in the LM method, and E is a unit matrix. Choosing for the initial condition $\mathbf{p}^0 = (p^0{}_n)$, $n \in N$, we define a new iteration for any iterative solution $\mathbf{p}^l = (p^l{}_n)$, $n \in N$, $l \geq 0$ as

$$\begin{gathered} \mathbf{p}^{l+1} = \mathbf{p}^l + [[A^l{}_{M0N}]^{\mathrm{T}} A^l{}_{M0N} + \mu_l E]^{-1} [A^l{}_{M0N}]^{\mathrm{T}} [(E_m{}^{ex}) - (E_m(\mathbf{p}^l))], \\ A^l{}_{M0N} := (\partial E_m(\mathbf{p}^l) / \partial p_n),\ m \in M_0,\ n \in N, \end{gathered} \tag{5.4}$$

where μ_l is a regularizing coefficient at each iteration step. The regularizing coefficient is chosen in the following way: if $f(\mathbf{p}^l) > f(\mathbf{p}^{l+1})$, then $\mu_{l+1} = \mu_l / 2$, otherwise $\mu_{l+1} = 2\mu_l$ until the condition of decrease of the functional is met.

The LM method is used conveniently with a fixed initial value of parameter μ_0, whose magnitude is taken at least an order of magnitude larger than the largest element of the $[A^l{}_{M0N}]^{\mathrm{T}} A^l{}_{M0N}$ matrix. In some standard programs one assumes even $\mu_0 = 10^4$. The value $\mu = 0$ is identified with the Gauss–Newton optimization method. The initial value of the parameter μ_0 can be related with the maximum and minimum diagonal values of matrix $[A^l{}_{M0N}]^{\mathrm{T}} A^l{}_{M0N}$. Thus, the LM method is considered as a one-parameter minimization algorithm whose parameter is the initial value of the regularizing coefficient. The initial conditions $\mathbf{p}^0 = (p^0{}_n)$, $n \in N$ for iterations of the kind of Eq. (5.4) can be derived from minimization of (4.5) for homogeneous (p_n), or from other considerations, e.g., technological estimates of the corresponding growth parameters. The criteria used to stop the minimization process were as follows

$$\begin{gathered} f(\mathbf{p}^l) < 10^{-12}, \\ (f(\mathbf{p}^l) - f(\mathbf{p}^{l+1})) / f(\mathbf{p}^l) < 10^{-2} \text{ for 5 iterations.} \end{gathered} \tag{5.5}$$

In some cases, the approach (5.4) converges very fast (quadratically) although only the first derivatives are used[43]. The number of necessary iterations is here smaller than that in the self-conjugated gradient method[45]. The rate of steps in the Gauss–Newton-type methods to which the LM method belongs is higher, because the time-consuming linear analysis of the goal function is not required here.

6. NUMERICAL EXPERIMENT IN THE EXAMPLE OF A TRAPEZOIDAL SI GRATING

To estimate the operating characteristics of the method developed and test the developed code, the following scheme of numerical experiment was composed. The ranges of the parameters to be found are, as a rule, known in advance (because they are determined by the technology used) and are a few tens of nanometers for linear dimensions and a few degrees for the angular ones. Within the above ranges, a set of parameters was specified (in a fairly arbitrary way), and the signature (the order efficiency vector) was calculated. For the initial value of parameters for the optimization procedure a vector randomly selected from those generated in the preceding steps was taken. Estimates of the parameters were obtained by the devised method, to be subsequently compared with the initial (preset) parameters. A comparison of the preset parameters with the estimates thus obtained yielded the accuracy of the parameter calculation.

In our particular example, a solid Si grating with a symmetrical trapezoidal profile and d = 1000 nm (see Fig. 2) was studied. The parameters of interest were found to be as follows: h = 1000 nm, b = 397.346 nm, and α = 80º. The Si refractive indices were taken from[46]. For the signatures we used data prepared in advance, which, because no measurements had been conducted in the first stage of the work, were obtained using the data of the exact calculational model based on the profile data selected in the region where the solution was looked for. The signature was calculated for 21 wavelengths λ in the 300 ÷ 800-nm interval, with 9 angles of incidence θ within the 0 ÷ 80º range, and two polarization states (TE and TM) in the –1, 0 and +1st reflected orders. The relative coordinates of the four points defining the vertices of the trapezoid served as parameters of the reconstruction. As the initial values of the parameters to be reconstructed served values chosen arbitrarily in the range under study. Tests were run with different values of the initial data. The optimization procedure was tested by choosing different values of μ_0 in the range from 10 to 1000.

Figures 4 and 5 present plots of order efficiency calculated for θ of 0 and 40º and exact reconstructable parameters vs. wavelength at the signature points. As follows from the figures, the order efficiencies vary noticeably under variation of λ, θ, and polarization, which suggests a possibility of using signatures of small length. Presented in Figs. 6 and 7 are the efficiencies of the 0th order in TE polarization obtained for the same angles of incidence but for eight sets of perturbed profile parameters (see data at the top of the figures). A comparison of different curves in these figures, as well as their comparison with the corresponding curves in Figs. 4 and 5, the efficiencies vary markedly under a relatively small

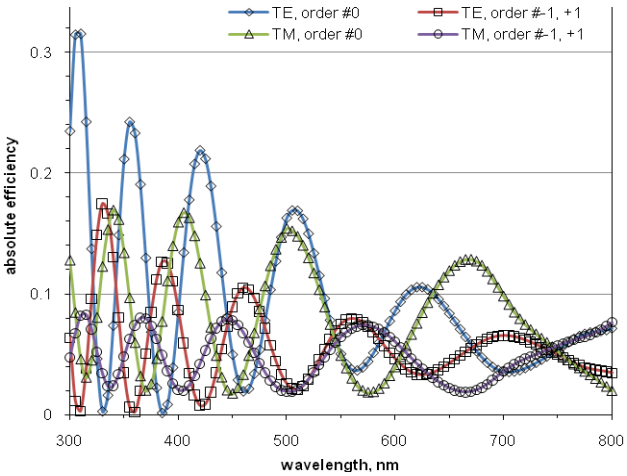

Figure 4. Efficiency of orders of a trapezoidal Si grating with the profile parameters to be reconstructed and $\theta = 0$, plotted vs λ.

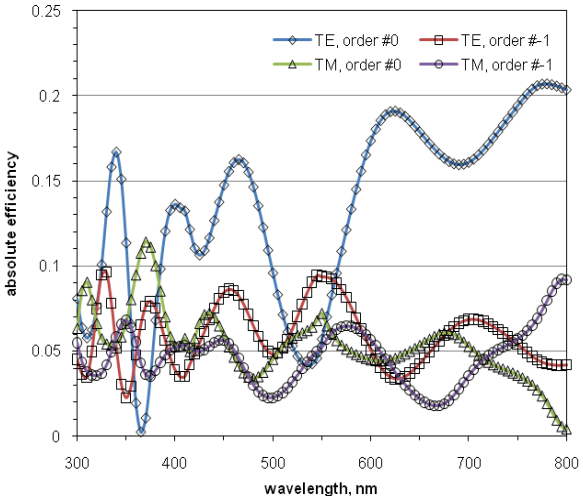

Figure 5. Efficiency of orders of a trapezoidal Si grating with the profile parameters to be reconstructed, $\theta = 40^{\circ}$, plotted vs λ.

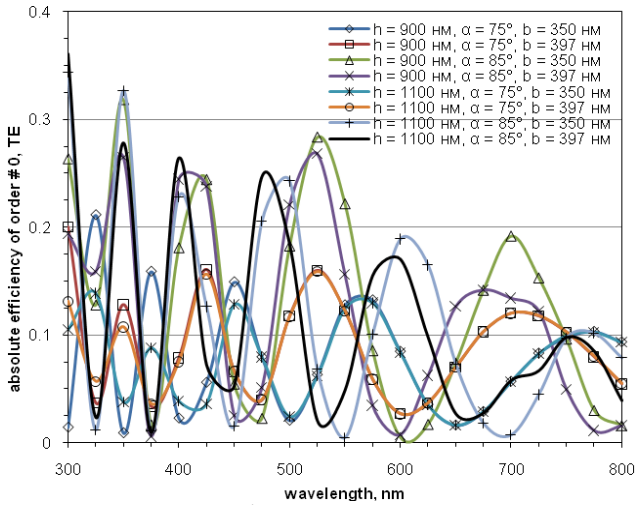

Figure 6. Efficiency of 0th order of a Si trapezoidal grating, with different profile parameters and $\theta = 0$, plotted vs. λ.

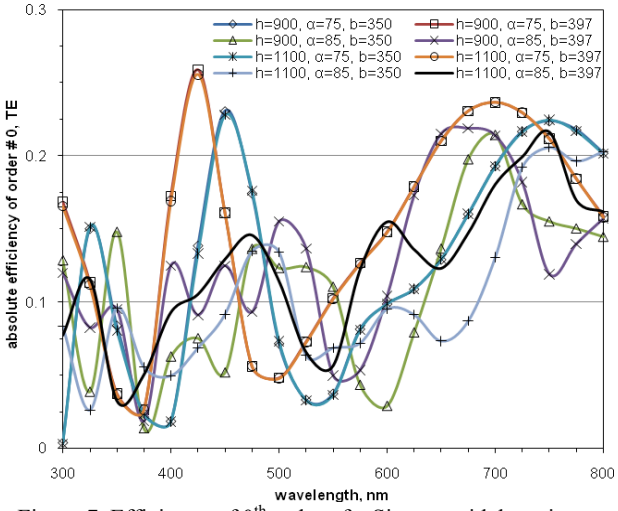

Figure 7. Efficiency of 0th order of a Si trapezoidal grating, with different profile parameters and $\theta = 40^{\circ}$, plotted vs. λ.

(within ±10%) variation of the profile parameters with respect to their unperturbed values. This observation, together with the monotonic character of their variations, suggests a fast and exact reconstruction of the parameters. Indeed, for all the nine sets of the parameters, the algorithm (5.4) locates in only 7–9 iterations the coordinates of the points with a relative accuracy (with respect to period) not worse than 10^{-6}, i.e., with an absolute accuracy of ~ 0.001 nm. For each signature, the algorithm was initiated 10 times with different initial data and the value of μ_0. Interestingly, it is approximately with the same accuracy that the direct solver calculates numerically the coordinates of boundary points, because it uses approximate relations to calculate the functions of the profiles and their derivatives. Apart from this, when the linear profile dimensions (coordinates of points) change by such a value, the efficiencies change by less than 10^{-6}, and this value is close to the maximum accuracy that can be reached in calculations with the direct solver in the case of smooth boundary functions. For non-smooth profiles, of the type of the trapezoid under consideration, the calculation accuracy is slightly worse.

The above model example is a fairly simple illustration of the optimization procedure developed and of the application of the MIM. This conclusion is supported by testing the dependence on the signature length. To obtain as accurate values of the reconstructed parameters, it will be sufficient to use a signature consisting only of nine values for θ and one order in one polarization. In this case, cond($[A^{ex}_{M0N}]^{T}A^{ex}_{M0N}$) of the matrix will be as large as a few thousand for different

realizations. The computing time in this case on a workstation with two Intel® Xeon® 2.66 GHz processors, 8 MB L2 Cache, 1333 MHz FSB, and 16 GB RAM, ~ 1–2 sec when operating on Windows Vista® Ultimate 64-bit and employing eightfold paralleling. As the signature length increases to 21 (for different λ), the condition number decreases to about a few hundred. Finally, for a signature with a full set of data (1134 long) it is about one hundred, but the computing time increases approximately 100 times.

7. CONCLUSION

The novel integral and nondestructive method of characterization of LDPAN structure by spectroscopic scatterometry in the UV–IR ranges is most appropriate, in the present author's opinion, for fast and comparatively low-cost measurements on instruments with a characteristic lateral size of components of ~ 10–100 nm, accuracy of their linear positioning of ~0.3 nm, and that of their angular location of ~ 0.1°. Due to the accuracy and broad range of possible applications which is inherent in the MIM chosen for solution of the direct diffraction problem, this approach can be readily applied to a broad variety of LDPAN classes, although in the present work some model constraints were imposed. In the cases where a complex 3D problem of diffraction from 2D gratings can be reduced to a 2D one from 1D grating or multilayer mirrors with plane boundaries, express or *in situ* analyses can be employed, which will permit one not only to determine the most important structural characteristics of LDPANs but to conveniently monitor the growth parameters of a sample. The latter aspect is a major prerequisite to producing instruments with preset and uniform optical and electronic properties.

The algorithm developed here for solution of a system of nonlinear operator equations with a limited set of unknown LDPAN structural parameters and a given set of known diffraction efficiencies needs further development, in particular, along the lines of broadening of the set and type of unknown parameters, selection of the optimum signature length, speeding up the process of solution in the case of slowly varying efficiency functions etc. There is also an obvious need of deep theoretical studies aimed at perfecting methods of regularization and control of the uniqueness and accuracy of a solution. While the computer code based on the gradient method of Löwenberg–Markwardt was found to be accurate enough and fast in solving a model problem for a trapezoidally profiled Si grating, the structure of real grown LDPANs turns out more complex for analysis. Further progress in the development of a method for solution of the inverse problem of diffraction from LDPANs, complemented by the availability of a large enough number of high-accuracy measurement data, permit one to hope that an effective solution of the general problem will eventually be found.

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