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Synthesis of perfectly conducting gratings with an arbitrary profile of slits

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Abstract. New approaches to solving the synthesis problem for a periodic grating from the incomplete set of scattering characteristics given in the frequency range or (and) on the interval of angles of incidence of plane waves are presented. These schemes are based on the idea of quasi-linearization of integral expressions of potential theory and allow one to obtain satisfactory results in long wavelength and, partially, in resonant (with respect to the grating sizes) ranges. The efficiency of the corresponding algorithms has been verified numerically.

1. Introduction

An investigation of dispersive properties of diffraction gratings [1, 2] has revealed a diversity of interesting phenomena from the standpoint of their practical implementation. However, the use of gratings as selective elements in resonance quasi-optical devices is substantially restricted by the complexity of the initial analysis of a designed unit. This analysis must meet two requirements. On the one hand, it has to take into account all key operating parameters of separate elements and, on the other hand, to judge the effectiveness of the system as a whole. This is the general problem of *model synthesis* in the design of resonance quasi-optical systems. The solution of this problem is divided naturally into the following conceptually independent steps. The first one is the construction of the electrodynamic model accounting for analytically an influence of scattering inhomogeneities varying in wave size. The second step consists in the analysis and parametric optimization of the electrodynamic model. The third step is the formation of the input data set for the synthesis of dispersive elements, such as gratings, and the last one is the solution of relevant inverse problems.

Here we present numerical algorithms for solving inverse boundary value problems for a perfectly conducting periodic grating with arbitrary height profile. The results are guided by key problems of the model synthesis of such resonance quasi-optical systems as efficiently absorbing and rescattering coatings, plane pattern-forming structures and open dispersive resonators with a considerably rarefied spectrum [3]. An analysis of the literature [4] shows that there is no reliable recommendation to progress in this direction. This fact determines the subject of our investigation. It is rare for gratings to come into the view of inverse problem

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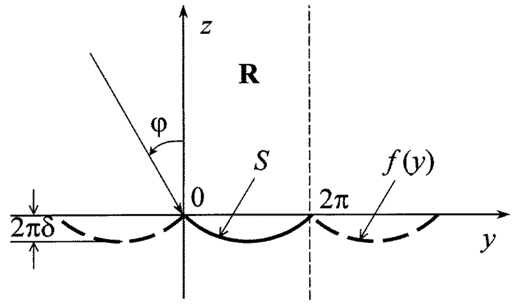

Figure 1. Geometry of the problem.

specialists. The number of important results in this field (see, for example, [5]) is not large, especially from the standpoint of the efficient solution of diversified applied problems.

2. Basic equations and formulation of the inverse problem

Let a grating (see figure 1, the structure is uniform in the x-direction) be illuminated by a plane E-polarized electromagnetic wave $U^p(y,z) = \exp[\mathrm{i}(\Phi_p y - \Gamma_p z)]$. Hereafter, $\Phi_p = p + \Phi$, $\Phi = \kappa \sin\varphi$, $\Gamma_p = (\kappa^2 - \Phi_p^2)^{1/2}$, $\operatorname{Re}\Gamma_p \geqslant 0$, $\operatorname{Im}\Gamma_p \geqslant 0$, $p = 0, \pm 1, \ldots$; κ is a dimensionless frequency parameter equal to the true grating's period to incident wavelength ratio, φ is an angle of incidence; S is a part of a periodic boundary, of period 2π, lying in the strip $\mathrm{R} = \{g : 0 \leqslant y \leqslant 2\pi\}$, $g = \{y, z\}$; $U^p = E_x$ is the only nonzero component of the electric field vector. We use dimensionless space–time coordinates wherein a period of the grating equals 2π and a time dependence factor is $\exp(-\mathrm{i}\kappa t)$. The solution $U(y,z)$ of the direct scattering problem everywhere in the strip R with the exception of the points of the boundary S can be represented as a single-layer potential [6, 7]

$$U(g) - U^p(g) = -\int_S \mu(g_0) G(g; g_0)\,\mathrm{d}g_0, \qquad g_0 = \{y_0, z_0\}, \tag{1}$$

where the continuous function $\mu(g_0)$ is a solution to the singular integral equation

$$\int_S \mu(g_0) G(g; g_0)\,\mathrm{d}g_0 = U^p(g), \qquad g \in S$$

and the Green function G is given by

$$G(g; g_0) = -(\mathrm{i}/4\pi) \sum_{n=-\infty}^{\infty} \Gamma_n^{-1} \exp\{\mathrm{i}[\Phi_n(y - y_0) + \Gamma_n |z - z_0|]\}.$$

Further assume that the boundary S is described by a single-valued function $f(y) : f(y) \leqslant 0$. Using the radiation condition [6]

$$U(g) = U^p(g) + \sum_{n=-\infty}^{\infty} a_{np} \exp[\mathrm{i}(\Phi_n y + \Gamma_n z)]$$

(a_{np} are complex amplitudes of harmonics of the diffraction spectrum) and the trivial condition

$$U(g) = 0 \qquad \text{for} \quad z < f(y)$$

we have from (1) that

$$\left\{ \begin{array}{c} a_{np} \\ -\delta_n^p \end{array} \right\} = (\mathrm{i}/4\pi\Gamma_n) \int_0^{2\pi} \eta(y_0) \left\{ \begin{array}{c} \exp[-\mathrm{i}\Gamma_n f(y_0)] \\ \exp[\mathrm{i}\Gamma_n f(y_0)] \end{array} \right\} \exp(-\mathrm{i}n y_0)\,\mathrm{d}y_0, \qquad n = 0, \pm 1, \ldots, \tag{2}$$

where

$$\eta(y_0) = \mu[y_0, f(y_0)]\{1 + [\mathrm{d}f(y_0)/\mathrm{d}y_0]^2\}^{1/2}\exp(-\mathrm{i}\Phi_0 y_0).$$

The inverse problem is to find the boundary S from the field $U(y, z)$ given exactly or not by the complex amplitudes $\{a_{np}\}$ in the region $z > 0$. The variety of inverse problems in electromagnetic theory of gratings is largely conditioned by the diversity of ways to form the input data set. (The calculation or measurement accuracy and the number of amplitudes, as well as the ranges of parameters κ and φ, can be chosen differently.) The classification of inverse problems (visualization, synthesis, parametric optimization) and the general questions associated with their well-posedness and solution (existence and uniqueness, linearization and regularization procedures) are discussed in [4, 5, 8, 9]. In [10] on the basis of equations (2) we construct closed algorithms for visualization (reconstruction) of $f(y)$ from fixed frequency (κ) and fixed illumination angle (φ) data. If the input data are complete and exact enough, the suggested algorithms ensure a satisfactory accuracy of the reconstruction for shallow surfaces (the profile depth is twice as large as wavelength λ) in the frequency range where a grating period is less than 4λ. The techniques developed in [10] are partially used below for solving the synthesis problem which is to determine the grating realizing the given complex amplitudes $a_{np}(\kappa, \Phi)$ (or close to them) in the given ranges of parameters κ and (or) Φ. The dimension of the input data set and the dimensionality of the integral equations (single, dual, etc) involving these data as the known part only are changed. Clearly there has to be a proper change in domains of the functions $a_{np}(\kappa, \Phi)$ (separate ranges of κ and Φ or their direct product), of integral operators, etc. So, rather than set forth the general situation we restrict the discussion to the case of fixed n and Φ. Then the problem is to synthesize a grating with the profile $z = f(y)$ such that the amplitude of the nth spatial spectrum harmonic differs little from $a_{n0}(\kappa)$, $\mathrm{Re}\,\Gamma_n(\kappa) > 0$ in the frequency range $[\kappa_1, \kappa_2]$.

3. Two synthesis algorithms

The first step is the same for both algorithms and consists in expanding the exponential functions $\exp[\mathrm{i}\Gamma_n f(y)]$ in the second relation (2) in power series. With only the highest terms in these series remaining we obtain

$$\eta(y, \kappa) \approx 2\mathrm{i}\Gamma_0. \tag{3}$$

Substituting (3) in the first equation of (2), we get the classical nonlinear problem (n is fixed)

$$a_{n0}(\kappa) = -(\Gamma_0/2\pi\Gamma_n)\int_0^{2\pi}\exp\{-\mathrm{i}[\Gamma_n\hat{f}(y) + ny]\}\,\mathrm{d}y, \qquad \kappa \in [\kappa_1, \kappa_2] \tag{4}$$

for the unknown function $\hat{f}(y)$ approximating $f(y)$, and we have to invert the Urysohn operator

$$A[f] = -(\Gamma_0/2\pi\Gamma_n)\int_0^{2\pi}\exp\{-\mathrm{i}[\Gamma_n f(y) + ny]\}\,\mathrm{d}y, \tag{5}$$

which is continuous from $\mathrm{C}[0, 2\pi]$ into $\mathrm{C}[\kappa_1, \kappa_2]$ ($\mathrm{C}[a, b]$ is the space of continuous functions defined on $[a, b]$).

We linearize the problem by means of functional differentiation. The Fréchet derivative of operator (5) at the point $g(y) \in \mathrm{C}[0, 2\pi]$ is the bounded linear operator $B_g : \mathrm{C}[0, 2\pi] \to \mathrm{C}[\kappa_1, \kappa_2]$, which can be written [11]

$$B_g[f] = (\mathrm{i}\Gamma_0/2\pi)\int_0^{2\pi}\exp\{-\mathrm{i}[\Gamma_n g(y) + ny]\}f(y)\,\mathrm{d}y.$$

Using the Newton–Kantorovitch algorithm, we reduce problem (4) to the determination of $\hat{f}(y) = \lim_{m\to\infty} f_m(y)$, where $\{f_m(y)\}$ is the sequence of solutions of the linear problems

$$B_{f_m}[f_{m+1}(y) - f_m(y)] = -A[f_m(y)] + a_{n0}(\kappa), \qquad m = 0, 1, 2, \ldots \tag{6}$$

or, in the simplified form,

$$B_{f_0}[f_{m+1}(y) - f_m(y)] = -A[f_m(y)] + a_{n0}(\kappa), \qquad m = 0, 1, 2, \ldots. \tag{7}$$

The bounded invertibility of the operators B_{f_m} and an appropriate choice for initial estimation $f_0(y)$ in iterative procedures are fundamental requirements to provide the convergence $f_m(y) \to \hat{f}(y)$ and the computational efficiency of the algorithms based on the inversion of equations (6) or (7) [11]. Since the required properties are not shared by the operators B_{f_m} (whose kernels are sufficiently smooth functions), it is necessary to regularize integral equations of the first kind (6) or (7).

Let us consider the integral operator $B_{f_m} : \mathrm{L}_2[0, 2\pi] \to \mathrm{L}_2[\kappa_1, \kappa_2]$ and the adjoint operator

$$B^*_{f_m}[a(\kappa)] = (\mathrm{i}/2\pi)\exp(\mathrm{i}ny)\int_{\kappa_1}^{\kappa_2} \Gamma_0 \exp[\mathrm{i}\Gamma_n f_m(y)]a(\kappa)\,\mathrm{d}\kappa.$$

By L_2 denote spaces of functions such that their moduli are square integrable. Assuming that the right-hand side of (6) does not belong to a nullspace of $B^*_{f_m}$, we obtain the equivalent problem

$$B^*_{f_m}B_{f_m}[f_{m+1}(y) - f_m(y)] = -B^*_{f_m}A[f_m(y)] + B^*_{f_m}[a_{n0}(\kappa)],$$
$$0 \leqslant y \leqslant 2\pi, \quad m = 0, 1, 2, \ldots. \tag{8}$$

Its operator is self-adjoint, positive, and compact from L_2 into L_2. It follows that the ill-posed operator equations of the first kind (8) can be replaced by the operator equations of the second kind by using the so-called Lavrent'ev regularization method (see, for example, [12]). The problem takes the form

$$(\alpha_m + B^*_{f_{m,\alpha}}B_{f_{m,\alpha}})[f_{m+1,\alpha}(y) - f_{m,\alpha}(y)] = -B^*_{f_{m,\alpha}}A[f_{m,\alpha}(y)] + B^*_{f_{m,\alpha}}[a_{n0}(\kappa)],$$
$$\alpha_m > 0, \quad 0 \leqslant y \leqslant 2\pi, \quad m = 0, 1, 2, \ldots, \tag{9}$$

where α_m are the regularization parameters. The solutions $f_{m,\alpha}(y)$ converge to $f_m(y)$ in the appropriate space norm as $\alpha_m \to 0$. The sequence $\{f_m(y)\}$, thus defined, gives the desired profile $\hat{f}(y)$ in the limit $m \to \infty$.

The equivalent reformulation and the regularization of problems (7) can be conducted similarly. The degree of convergence $f_m(y) \to \hat{f}(y)$ in this case is lower [11]. However, the advantages resulting from the statistical character of the operator B_{f_0} are worthy of notice. We have to invert B_{f_0} properly only once. Without going into details and assuming $f_0(y) \equiv 0$ let us write at once

$$\alpha[f_{m+1,\alpha}(y) - f_{m,\alpha}(y)] + \gamma_1 \exp(\mathrm{i}ny)\int_0^{2\pi} \exp(-\mathrm{i}ny_0)[f_{m+1,\alpha}(y_0) - f_{m,\alpha}(y_0)]\,\mathrm{d}y_0$$
$$= \gamma_2(m, \alpha, y), \tag{10}$$

where

$$\gamma_2(m, \alpha, y) = (\mathrm{i}/4\pi^2)\exp(\mathrm{i}ny)\int_{\kappa_1}^{\kappa_2} (\Gamma_0^2/\Gamma_n)\left\{\int_0^{2\pi} \exp\{-\mathrm{i}[\Gamma_n f_{m,\alpha}(y_0) + ny_0]\}\,\mathrm{d}y_0\right\}\mathrm{d}\kappa$$
$$+ (\mathrm{i}/2\pi)\exp(\mathrm{i}ny)\int_{\kappa_1}^{\kappa_2} \Gamma_0 a_{n0}(\kappa)\,\mathrm{d}\kappa,$$
$$\gamma_1 = (1/4\pi^2)\int_{\kappa_1}^{\kappa_2} \Gamma_0^2\,\mathrm{d}\kappa, \qquad m = 0, 1, 2, \ldots, \quad \alpha > 0, \quad 0 \leqslant y \leqslant 2\pi.$$

The kernels of integral equations of the second kind (10) are degenerate. This allows us to give the solution in an explicit form

$$\alpha[f_{m+1,\alpha}(y) - f_{m,\alpha}(y)] = \gamma_2(m,\alpha,y) - \gamma_1\gamma_3(m,\alpha)(\alpha + 2\pi\gamma_1)^{-1}\exp(\mathrm{i}ny), \quad \alpha > 0,$$
$$\gamma_3(m,\alpha) = \int_0^{2\pi} \exp(-\mathrm{i}ny)\gamma_2(m,\alpha,y)\,\mathrm{d}y. \tag{11}$$

Let $\alpha \to 0$. Calculating the sequence $\{f_m(y)\}$ for growing m we arrive at the desired $\hat{f}(y)$.

4. The problem of initial approximation and numerical results

One possibility to choose the initial value $f_0(y)$ in iterative procedures have already been realized in (7), (10), and (11). However, on the whole, this question remains open (in the inversion of nonlinear problem (4)) and calls for certain efforts for its satisfactory resolution. The scheme below is more crude, but it is self-closed and can be useful both in solving synthesis problems and in obtaining 'good' estimations $f_0(y)$. The essence of the algorithm is as follows: n and Φ are considered fixed as before, the formulation of the inverse problem remains unchanged. Representation (3) is used in the second equation of system (7) from [10] $(N = 1)$, which has to be inverted with respect to the unknown function $\hat{f}(y)$. The resulting integral equation of the first kind

$$a_{n0}(\kappa) + \delta_n^0 = (\mathrm{i}\Gamma_0/\pi)\int_0^{2\pi} \hat{f}(y)\exp(-\mathrm{i}ny)\,\mathrm{d}y, \qquad \kappa \in [\kappa_1, \kappa_2]$$

is reduced to the integral equation of the second kind

$$\alpha\hat{f}_\alpha(y) + \exp(\mathrm{i}ny)(\kappa_2 - \kappa_1)\int_0^{2\pi}\exp(-\mathrm{i}ny_0)\hat{f}_\alpha(y_0)\,\mathrm{d}y_0 = -\mathrm{i}\pi\exp(\mathrm{i}ny)\int_{\kappa_1}^{\kappa_2}\Gamma_0^{-1}[a_{n0}(\kappa) + \delta_n^0]\,\mathrm{d}\kappa, \qquad 0 \leqslant y \leqslant 2\pi \tag{12}$$

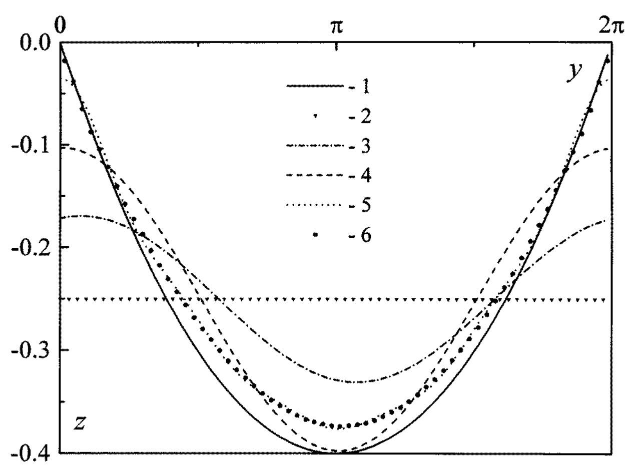

Figure 2. Control profile (full curve 1) and synthesized profiles (curves 2–6) for different input data sets. 2: $M = 1$. 3: $M = 2$. 4: $M = 3$. 5: $M = 11$. 6: $M = 31$. M is the number of exact scattered amplitudes $a_{n_1,0}, \ldots, a_{n_M,0}$ of the control structure included in the input data set for the synthesis problem.

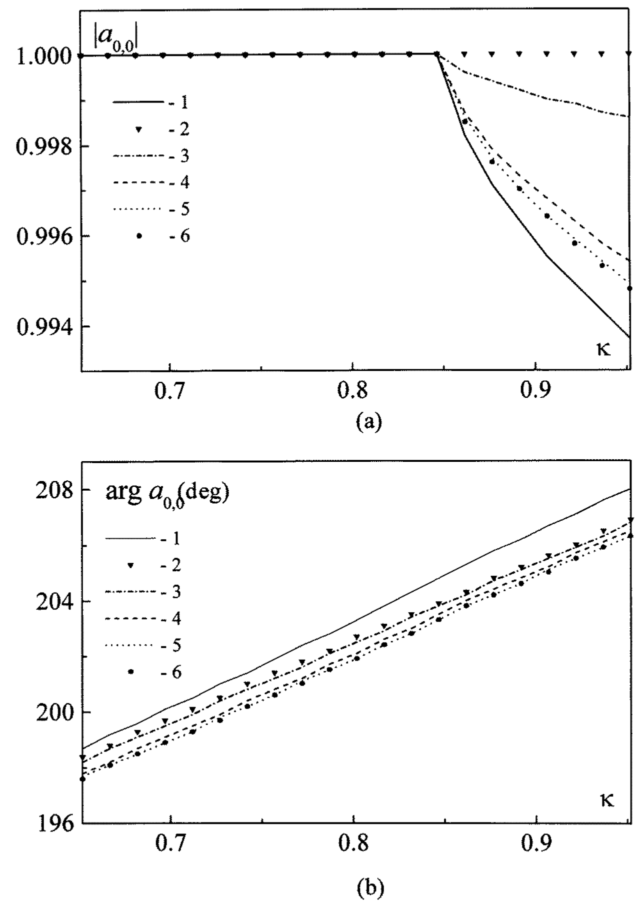

Figure 3. Absolute value (*a*) and argument (*b*) of the diffraction spectrum amplitude $a_{0,0}(\kappa)$ for control (full curves 1) and synthesized (curves 2–6) gratings. Curves 2–6 correspond to different input data sets. 2: $M = 1$. 3: $M = 2$. 4: $M = 3$. 5: $M = 11$. 6: $M = 31$.

by using the Lavrent'ev regularization method. The solution $\hat{f}_\alpha(y)$ exists, is unique, and tends to $\hat{f}(y)$ as $\alpha \to 0$ ($\|\hat{f}_\alpha(y) - \hat{f}(y)\|_{L_2} \to 0$ as $\alpha \to 0$). The kernel of the integral operator in (12) is degenerate, therefore the function $\hat{f}_\alpha(y)$ can be written in an explicit form. It is coincident with (11) up to notation.

The case when M scattered amplitudes $a_{n_1,0}, a_{n_2,0}, \ldots, a_{n_M,0}$ in the frequency range are given is more frequent in applied problems. The technique used in this situation is identical to that for $M = 1$. Without going into details let us write the final formula:

$$\hat{f}(y) = \mathrm{Re}\left\{[2\mathrm{i}\Gamma_0(\kappa_2 - \kappa_1)]^{-1} \int_{\kappa_1}^{\kappa_2} \sum_{m=1}^{M} (a_{n_m,0} + \delta_{n_m}^0) \exp(\mathrm{i}my)\, \mathrm{d}\kappa\right\}. \qquad (13)$$

Figures 2–5 illustrate the numerical results of synthesis of the grating realizing the given amplitudes $a_{n_m,0}(\kappa)$ in the frequency range $0.652 \leqslant \kappa \leqslant 0.952$ with $\varphi = 10^\circ$. We take the requirements imposed upon the synthesized structures from the solution of the direct scattering problem. The method employed (the analytical regularization method [6, 13]) is based on the idea of analytical inversion of the singular part of a boundary integral equation of potential theory (see section 2) and reduces the initial ill-posed problem to the Fredholm infinite system

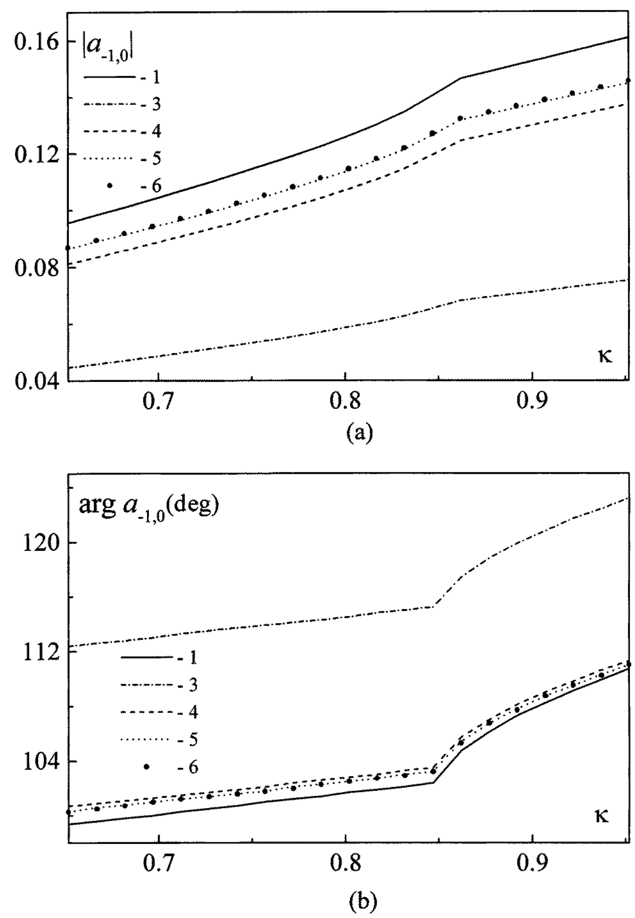

Figure 4. Same as figure 3 except the illustration is given for the amplitude $a_{-1,0}(\kappa)$.

of linear algebraic equations. The properties of the matrix operator of this system allow the use of a rapidly converging (in the norm of one of the spaces of infinite sequences) reduction method. The control profile (see figure 2) and the relevant scattering characteristics (see figures 3–5) are depicted by the full curves 1. The dotted and broken curves 2–6 are profiles of synthesized structures and their scattering characteristics. The curves 2–6 correspond to the sets of the input data $\{a_{0,0}(\kappa); M = 1\}$, $\{a_{-1,0}(\kappa), a_{0,0}(\kappa); M = 2\}$, $\{a_{\pm1,0}(\kappa), a_{0,0}(\kappa); M = 3\}$, $\{a_{-5,0}(\kappa), a_{-4,0}(\kappa), \ldots, a_{5,0}(\kappa); M = 11\}$, and $\{a_{-15,0}(\kappa), a_{-14,0}(\kappa), \ldots, a_{15,0}(\kappa); M = 31\}$, respectively. We can estimate the result as wholly satisfactory. The fulfilment of requirements is in reasonable error, we can predict the dynamics in transformation of synthesized profiles as M increases. These changes are consistent with the statement (see [4]) about the uniqueness of the inverse problem solution in the case of a complete set of exact input data. Note that M in the numerical example is not an iterative process variable. Each M determines its own problem with its distinctive set of features required of the synthesized structure. Figures 2–5 allow us to judge the accuracy of the fulfilment of these requirements in the framework of the algorithm. For a correct comparative estimation of the accuracy we must take account of the arguments and the absolute values of the amplitudes $a_{n,0}(\kappa)$ on the whole interval $[\kappa_1, \kappa_2]$ for all significant values of n. An examination of just one fragment (for example, the fragment

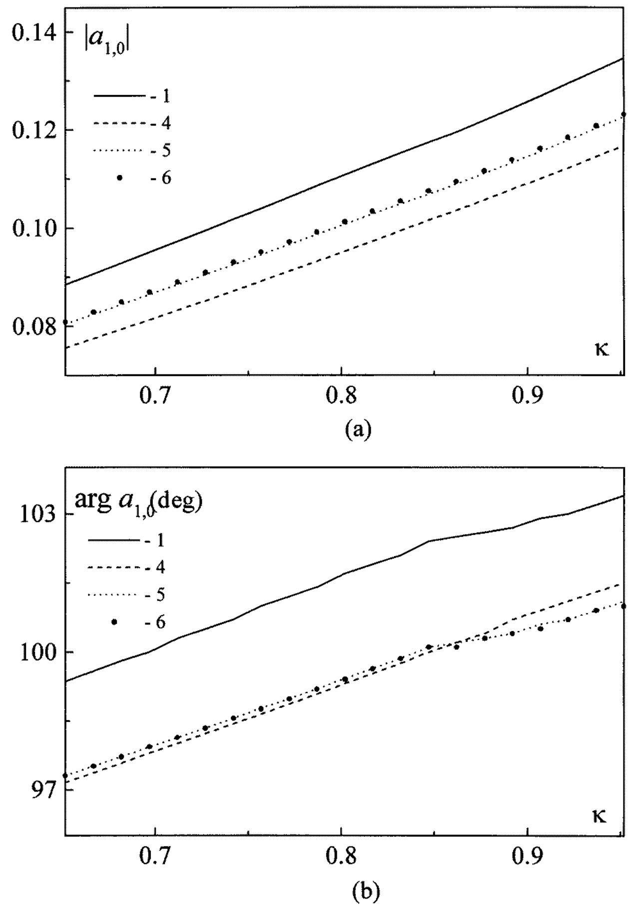

Figure 5. Same as figure 3 except the illustration is given for the amplitude $a_{1,0}(\kappa)$.

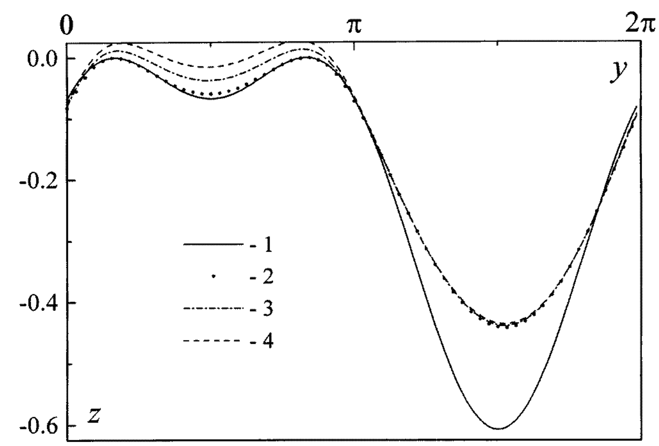

Figure 6. Control profile (full curve 1) and synthesized profiles (curves 2–4) for different levels of distortion of the input data.

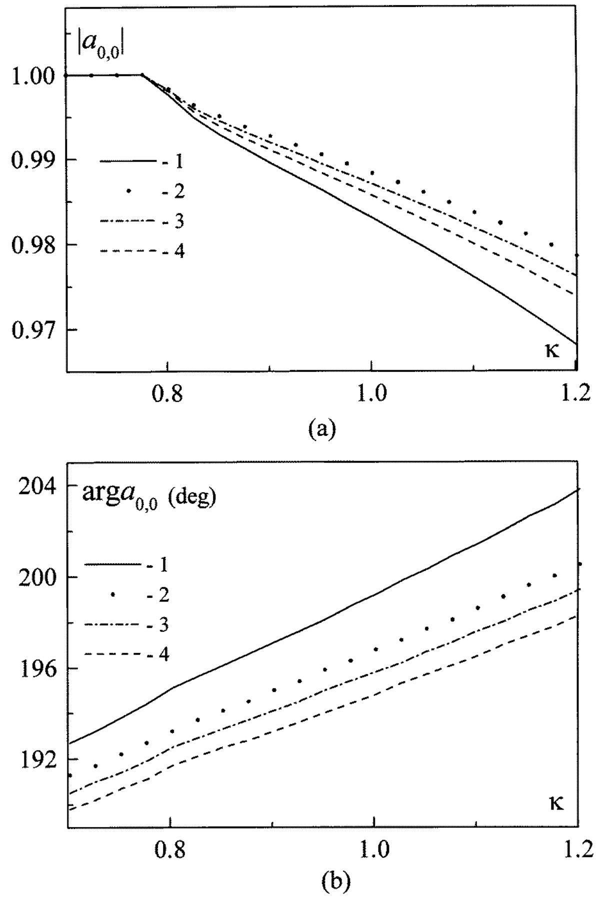

Figure 7. Scattering characteristics of the control (full curve 1) and synthesized (curves 2–4) structures.

from figure 3(*b*) where the characteristic $\arg a_{0,0}(\kappa)$ for synthesized structures deviates from the desired one) is inadequate to formulate the conclusions.

The sequence of the resolved synthesis problems can be considered as the solution of the profile reconstruction problem with an incomplete set of exact input data. (The completion is achieved by a growth of M.) Since the reconstruction problem is stated in a frequency range, the solution must converge to the real profile as M is sufficiently large [4, 8, 9]. Figures 2–5 confirm the 'internal' convergence of the method (curves 5 and 6 merge together almost everywhere), yet show a minor difference between the reconstructed (the result for $M = 31$) and the real profile. (The error is up to 6% in a uniform metric for profiles.) This rather regular error is stipulated by the approximation of the algorithm. The less the relative grating height, the less the error [10]. It can be reduced substantially by the use of two basic algorithms described above. The numerical example presented here concerns in essence the problem of choosing the initial estimation in these schemes. However, the characteristics of the obtained solution allow us to use it not only as a 'good' initial estimation $f_0(y)$ in nonlinear problem (4), but also as a final or intermediate result in the relevant synthesis problems or in the reconstruction problems with an incomplete set of exact input data.

A few words about the robustness of the algorithm with respect to faint noise in the input data. Random deviations of the values $a_{n,0}(\kappa)$ from the exact values to within 10% do not introduce large errors into the synthesis or reconstruction problem solution. This is supported by the results of the numerical experiment presented in figures 6 and 7. The problems are solved in the frequency range $0.702 \leqslant \kappa \leqslant 1.202$ with $\varphi = 15^\circ$ for the control profile $f(y) = 0.27(\sin y + \cos^2 y - 1.25)$. The set of the input data is $\{a_{-10,0}(\kappa), a_{-9,0}(\kappa), \ldots, a_{10,0}(\kappa); M = 21\}$. Curves 1 are the control grating and its scattering characteristics, curves 2–4 are the synthesized structures and their scattering characteristics. Curves 2 correspond to the exact input data, curves 3 and 4 correspond to the input data distorted randomly within 5% and 10%, respectively.

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