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SCALAR AND ELECTROMAGNETIC PROPERTIES OF X-RAY DIFFRACTION GRATINGS

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Limitations of the scalar diffraction theory when analyzing the X-ray grating efficiency were determined. The necessity to use vector electromagnetic approaches was shown. A new non-scalar property was described, which was inherent to the efficiency behavior of high-frequency X-ray gratings of any profile and manifested itself, when a grating coating material was changed. Efficiency curves calculated by exact integral equations and measured using synchrotron radiation were compared.

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1. Introduction

The use of X-ray diffraction gratings are most promising in short-wavelength optics; however, their efficiency simulation using rigorous methods is complicated in comparison with calculations in other ranges [1]. For example, a rigorous analysis based on the differential method was presented in [2] *for only an ideal sawtooth* profile with a small number of layers and only in TE polarization. At the same time, the scalar diffraction theory or perfect conductivity approximation do not provide accurate results, especially at grazing angles of incidence, in TM polarization, and for high frequencies and grating orders [1].

Based on the integral equation method developed by the author, referred to as the modified one [3,4], some conclusions of the scalar approximation are analyzed, its errors are determined, and a new electromagnetic property in the behavior of the absolute efficiency of X-ray gratings are described in this paper.

2. Conclusions of the scalar diffraction theory

An important feature of X-ray gratings is small ratios of the wavelength λ and the line depth h to the period d. The grating operates in the scalar mode if $\lambda/d < 0.2$ at $h/d < 0.1$ and angles of incidence and diffraction are close to normal. Under grazing incidence at $\lambda/d < 0.1$ and even < 0.05, this approximation is unacceptable [1].

The scalar mode is characterized by the absence of polarization effects and anomalies, and the efficiency of perfectly reflecting gratings is determined from universal curves plotted for the various line profiles [1]. The universal curve is a unique function of the ratio h/d and is valid for gratings with various periods, line depths, and materials.

In [5], the absolute efficiency $E^{\mathrm{a}}_{\mathrm{m}}(n)$ of a multilayer X-ray grating in the order n was considered as the product of the reflectance $R_{\mathrm{m}}(\theta')$ of a plane multilayer mirror and the efficiency $E^{\mathrm{p}}(n,\theta)$ of the perfectly reflecting grating,

$$E^{\mathrm{a}}_{\mathrm{m}}(n) = R_{\mathrm{m}}(\theta')\, E^{\mathrm{p}}(n,\theta), \tag{1}$$

where the angle of incidence $\theta = \theta'$ in the general case and $\theta = \theta' + \delta$ for a sawtooth grating with the blaze angle δ.

For the sawtooth profile, instead of the rigorously calculated efficiency of the perfectly reflecting grating, the phenomenological formula based on geometrical concepts [1,6] can be used,

$$E_{\mathrm{m}}^{\mathrm{a}}(n) = R_{\mathrm{m}}(\theta - \delta)\ \min\Big[\cos(\theta - 2\delta)/\cos\theta,\ \cos\theta/\cos(\theta - 2\delta)\Big]. \tag{2}$$

The feature of these operating conditions is that waves incident and diffracted into the nth order are symmetric with respect to the normal to the operating line face, which provides the grating blaze. However, even at the high relative efficiency of the blaze grating (typically about 90 %), its absolute efficiency is low near autocollimation for the short wavelengths. The necessity to increase the efficiency of X-ray gratings requires the use of grazing angles of incidence or/and multilayer coatings, and the scalar theory becomes unacceptable.

3. Limitations of the scalar theory and achievements of rigorous vector approaches

A fundamental limitation of the above-described scalar approach for continuous and multilayer gratings is the angle of incidence which should not be too grazing. It is believed that the angle of incidence should not exceed 40° for continuous gratings [5]. It was found that scalar efficiency (2) differs from the efficiency calculated on the basis of the rigorous differential method [5] for a multilayer grating operating at an angle of incidence of 45°. However, the critical angle depends on the grating parameters, light wavelength, and polarization. The angle of incidence, at which rule (1) is satisfied, can be increased to 70–80° in some cases [2]. The limitation to the angle of incidence is caused by different efficiencies of finitely and perfectly conducting continuous X-ray gratings at grazing incidence, especially in TM polarization [1]. The same is also observed for multilayer gratings if light reaches a substrate.

Rigorous calculations based on differential, integral, and modal methods showed that the absolute efficiency of the continuous X-ray grating changes unpredictably, from the viewpoint of the scalar theory, as the line configuration and frequency, the angle of incidence, and the wavelength vary [3, 7, 8]. The error of the determination of optimal grating and radiation parameters on the basis of simple phenomenological expressions increases when the grating frequency and order, the angle of incidence, and the wavelength increase.

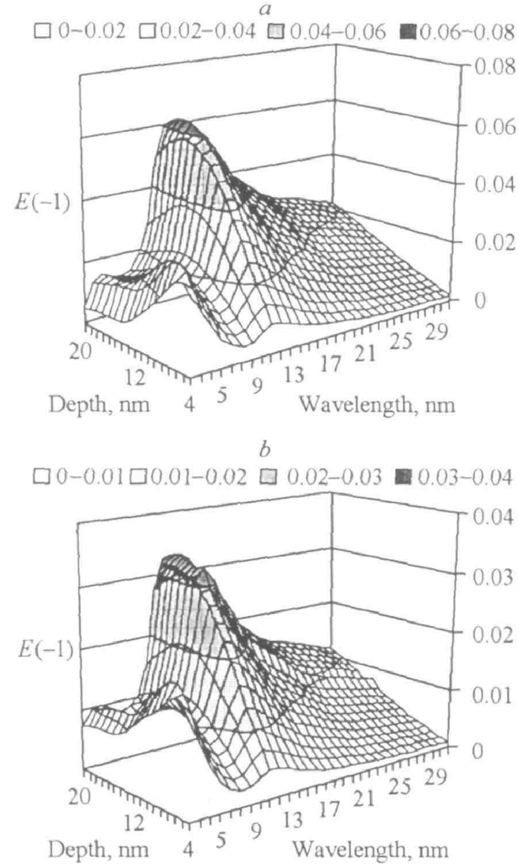

Figure 1. Absolute 3D efficiency of the minus first order in unpolarized radiation of the gold sinusoidal grating with a period of 3600 line·mm^{-1} at angles of incidence of 88 (a) and 89° (b) as a function of the depth and wavelength.

Let us demonstrate the possibility of a rigorous numerical analysis of the efficiency in a wide range of parameters by the example of a gold sinusoidal grating with a period of 3600 line·mm^{-1}, operating in unpolarized radiation with a wavelength of 1 to 30 nm at angles of incidence of 88 and 89°. To determine the optimal parameters and efficiency of the grating with the refractive index of gold [9], scanning over several parameters was used. A subroutine of this procedure was an electromagnetic calculation based on the modified integral equation method [4]. The nonscalar behavior of the efficiency for this example becomes especially notable at angles of incidence larger than 80°. The optimal scalar depth differs from the exact one (Fig. 1) by 15 % for an angle of 88° and by 20 % for 89°. The scalar efficiencies at the peak differ from rigorously calculated ones by 133 and 146 %, respectively. Spectral curves in the short-wavelength range for various depths have two pronounced and comparable in height peaks, which are not predicted by the scalar theory (Fig. 1). The first and second peaks are caused by an increase in the reflectance and the blaze (resonance) of the grating line profile, respectively. The efficiency curves near peaks and in the long-wavelength edge also significantly differs from typical scalar curves. High-order efficiencies predicted by the scalar theory can differ by tens of times from the results of rigorous calculations [10].

In [7], it was concluded that the single simple prediction which can be made is the replacement of the grating material. If all other grating and radiation parameters remain unchanged, the absolute efficiency will change according to the ratio of material reflectances. Thus, it is argued in [7] that expressions (1) and (2) can be applied to any parameters of the continuous grating and light. Numerous rigorous calculations carried out by the author confirm the high accuracy of expressions (1) and (2) only for gratings with periods of 300 and 600 line·mm^{-1} [11,12].

4. New electromagnetic property of the efficiency and its manifestation

The inaccuracy of the conclusion of [7], that was revealed using the rigorous integral method, allowed us to find and to study a new scalar property inherent to the variation in the efficiency of high-frequency X-ray gratings, including multilayer ones, which manifests itself for all profile types [11,12]. For simplicity, let us formulate this property for continuous gratings, bearing in mind its identity for multilayer gratings, if radiation reaches a substrate. If the line parameters, angle of incidence, and wavelength are unchanged, but the refractive index n of a material of the high-frequency grating is replaced, it is impossible to determine its new efficiency at the nth order peak by multiplying its previous value by the ratio of the Fresnel reflectances,

$$E(n,\tilde{n}_2) = E(n,\tilde{n}_1)\, R_{\mathrm{F}}(\tilde{n}_2)/R_{\mathrm{F}}(\tilde{n}_1). \qquad (3)$$

Expression (3) is a generalization of phenomenological formula (2) for the continuous grating with any profile and it means the following. If the relative grating efficiency controlled by the line profile is known, the absolute efficiency is equal to the product of the relative efficiency and the Fresnel reflectance calculated for a certain angle of incidence. The nonscalar effect and inaccuracy of expressions (2) and (3) notably manifest themselves only for high-frequency gratings and include two aspects. First, it is impossible to predict the absolute efficiency of the grating using the ratio of coating material reflectances when replacing the grating material. Second, the optimal parameters of radiation and line profile shape (the angle of incidence, wavelength, line depth, angles for the triangular profile, porosity for a lamellar profile, and others), determined for one grating material are not optimal for another.

Table 1 lists the results of rigorous calculation of the grating efficiency for three basic profile types of various frequency with the refractive indices of gold $\tilde{n}_1$ and $\tilde{n}_2$ [12]. The radiation and grating parameters optimal for a wavelength of 4.4 nm and refractive index $\tilde{n}_1$ were used in the calculation. In Table 1, the first column contains the ratios of efficiencies, obtained with refractive indices $\tilde{n}_1$ and $\tilde{n}_2$ for each profile type, the second column includes ratios of corresponding Fresnel reflectances. The error of formulas (2) and (3) for low-frequency gratings with 300 and 600 line·mm^{-1} is several percent, which justifies their application. For gratings with periods of 2400 and 3600 line·mm^{-1} of any profile, the error of formulas (2) and (3) reaches 30 to 35 %, which is very significant, since the efficiencies themselves are low. The incorrectness

Table 1. $E(-1, \tilde{n}_2)/E(-1, \tilde{n}_1)$ and $R_{\mathrm{F}}(\tilde{n}_2)/R_{\mathrm{F}}(\tilde{n}_1)$, where $\tilde{n}_1 = 0.9942 + i0.0058$, $\tilde{n}_2 = 0.9896 + i0.0096$, $\lambda = 4.4\,\mathrm{nm}$.

F, mm^{-1}	Sinusoidal grating		Sawtooth grating		Lamellar grating	
	$\frac{E(-1,\, \tilde{n}_2)}{E(-1,\, \tilde{n}_1)}$	$\frac{R_{\mathrm{F}}(\tilde{n}_2)}{R_{\mathrm{F}}(\tilde{n}_1)}$	$\frac{E(-1,\, \tilde{n}_2)}{E(-1,\, \tilde{n}_1)}$	$\frac{R_{\mathrm{F}}(\tilde{n}_2)}{R_{\mathrm{F}}(\tilde{n}_1)}$	$\frac{E(-1,\, \tilde{n}_2)}{E(-1,\, \tilde{n}_1)}$	$\frac{R_{\mathrm{F}}(\tilde{n}_2)}{R_{\mathrm{F}}(\tilde{n}_1)}$
300	1.238	1.179	1.263	1.253	1.222	1.168
600	1.328	1.202	1.338	1.327	1.285	1.155
1200	1.519	1.217	1.570	1.518	1.556	1.202
2400	1.917	1.274	1.692	2.038	1.892	1.274
3600	1.955	1.313	1.689	2.532	1.870	1.320

Table 2. $E(-1, \tilde{n})$, h_{opt}, and θ_{opt} for the sinusoidal grating with $3600\,\mathrm{line{\cdot}mm^{-1}}$, $\lambda = 12.8\,\mathrm{nm}$.

	Material	h, nm	θ, deg	$E(-1, h_i, \theta_i)$	$E(-1, h_j, \theta_j)$	$E(-1, h_k, \theta_k)$
i	Au	15.25	79.2	0.1500	0.1387	0.1302
j	F-1 glass	17.75	82.0	0.0301	0.0354	0.0343
k	Al	17.0	83.2	0.0232	0.0277	0.0287

of the conclusion [7] makes impossible, in particular, the use of known formula (2) to calculate the efficiency of high-frequency X-ray gratings with a sawtooth profile.

Let us consider the influence of the detected electromagnetic effect which is caused by the finite conductivity of a material of high-frequency gratings on their optimal parameters. Optimal parameters of high-frequency gratings cannot be determined from simple geometrical considerations. However, it is not clear if the optimal parameters determined by numerical calculation remain optimal when grating material is replaced. Table 2 lists the rigorously calculated optimal parameters for a wavelength of 12.8 nm and maximum efficiencies in TE polarization of the sinusoidal grating with a period of $3600\,\mathrm{line{\cdot}mm^{-1}}$, prepared from various materials such as gold, aluminum, and flint glass [12]. The optimal angles of incidence and grating coating depths for various materials are listed on the left-hand side of Table 2. The right-hand side contains the efficiencies of the minus first-order grating with optimal (diagonal terms) and nonoptimal (nondiagonal terms) parameters, which are optimal for another material. When using a grating with parameters optimized for operation with one coating material, replacement of the latter by another material decreases the efficiency by several tens of percent in comparison with the maximum attainable one.

Let us demonstrate the detected nonscalar property using the example of spectral curves of the minus first-order efficiencies of gold and aluminum sinusoidal gratings with $3600\,\mathrm{line{\cdot}mm^{-1}}$, optimized for operation at a wavelength of 12.8 nm in TE polarization with the parameters taken from Table 2. Figure 2 shows four spectral curves of the grating efficiency in the soft X-ray range, two of which were calculated with optimal parameters, and two others with nonoptimal parameters which are optimal for another material. The efficiencies of gratings with nonoptimal parameters differ from those calculated with optimal parameters by tens of percent near the peak and by several times at the edges of the range.

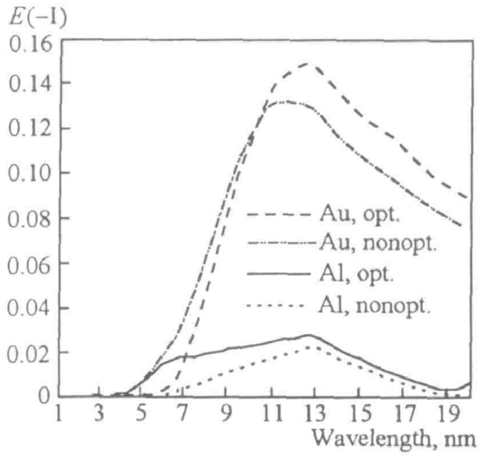

Figure 2. Spectral efficiency of the minus first order in TE polarization of gold and aluminum sinusoidal gratings with a period of 3600 line·mm^{-1} for parameters optimal and nonoptimal for a given material at a wavelength of 12.8 nm.

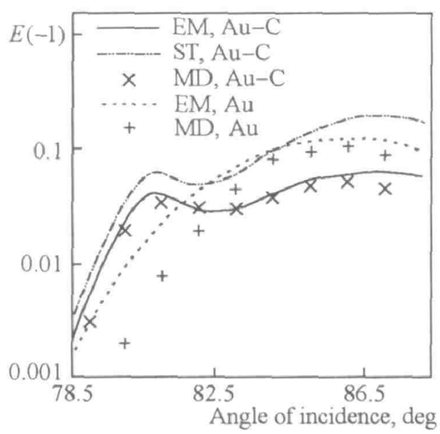

Figure 3. Absolute efficiency of the minus first order in TE polarization of gold and multilayer (three Au–C pairs) sawtooth gratings with a blaze angle of 1.5° and a period of 1200 line·mm^{-1} as a function of the angle of incidence at a wavelength of 5 nm; electromagnetic calculation (EM), scalar theory calculation (ST), and measured data (MD).

As an example of the electromagnetic behavior (not described by relation (1)) of the multilayer grating efficiency, a gold grating with sawtooth profile, a blaze angle of 1.5°, and a period of 1200 line·mm^{-1} was taken. The grating was coated with three pairs of gold–carbon layers optimized in thickness to increase the efficiency at operating points of a Bumble Bee monochromator used in the Doris storage ring [13]. The minus first-order efficiency in TE polarization was measured using fixed lines obtained by the monochromator. The calculated efficiencies of the multilayer grating, obtained for a wavelength of 5 nm using the integral method [4], agree well with the measured values in the entire range of grazing angles (Fig. 3). The scalar approximation yields values that differ significantly from the experimental ones, especially in the wide-angle range. A certain difference between the experimental and theoretical data is caused by the use of the perfect line profile in the model, which is confirmed by comparison of the measured efficiencies of the continuous gold grating and those calculated by the electromagnetic theory (Fig. 3).

5. Conclusion

Finally, let us briefly formulate the most important conclusions and possible directions of this study. The scalar theory cannot adequately predict the behavior of the absolute efficiency of practical X-ray gratings operating even near normal incidence. On the contrary, rigorous electromagnetic numerical calculation readily yields both accurate values of the absolute efficiency and the optimal parameters of radiation and gratings. For the high-frequency grating, a coating material replacement requires recalculation of the efficiency and optimal parameters of the grating and radiation using rigorous methods. To attain a high-accuracy agreement with the measured data, actual boundary profiles (for example, measured using atomic-force microscopy [4]) should be used in the calculation, as well as refractive indices appropriate for the range under study [9, 14]. A more adequate consideration of random roughnesses of boundaries and interdiffusion of layers requires further development of the used model [4].

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