Electromagnetic solution for scattering from 2D rough surfaces through general solutions for 1D rough surfaces in short waves

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The paper reports on the electromagnetic solution of scattering from 2D rough surfaces in short waves using boundary integral equations for conical diffraction and Monte Carlo simulations. The general equivalence rule for determination of the efficiencies of reflected orders of bi-gratings from those calculated for classical gratings is derived. The mean differential reflection coefficient of a rough mirror working at an x-ray wavelength under grazing incidence has been computed for the first time using the equivalence formulae.

1 Introduction

Multi-wave and multiple diffraction, refraction, absorption, waveguiding, and wave deformation govern to a considerable extent scattering of x-ray and extreme ultraviolet radiation and cold neutrons from nanoroughness of continuous media. Inclusion of these pure dynamic effects, which requires application of electromagnetic theory, permits one to calculate the absolute intensity of the specular component and describe adequately the intensity distribution of the diffuse component which may have resonance peaks. Some surfaces are deterministic, e.g., perfect gratings, and some are random, e.g., polished mirrors. Some surfaces are 1D, e.g., classical gratings with one-dimensional periodicity (1D gratings) and cutting mirrors, but most are 2D, e.g., bi-periodic gratings (bi-gratings or 2D gratings), ocean surfaces, and surfaces with atomic scale roughness. Any number of possible combinations between these four characteristics may be present in real structures, e.g., 1D gratings with 2D random roughness. Despite the impressive progress reached recently in development of exact numerical methods of investigation of wave diffraction from boundary roughness [1,2], the present author is aware only of asymptotic and perturbation approaches to the analysis of x-ray and cold neutron scattering for 2D rough surfaces, such as the scalar Kirchhoff integral, parabolic wave equation, Rayleigh method, Born approximation, distorted-wave Born approximation, and a few others [3, 4].

It is well-known that solution of the 2D and 3D Helmholtz equations with any rigorous numerical codes meets with difficulties at high ratios of characteristic dimension to wavelength λ. The rigorous modified method of boundary integral equations (MIM) [4, 5] has been widely employed in analyzing the efficiency of bulk and multilayered diffraction gratings, including but not restricted to those in x-rays and conical mounts [6]. The approach is very accurate and fairly fast convergent in the range of very small ratios of λ to period d and groove depth h, particularly for structures with real (measured or obtained from a growth model) boundary profiles [7]. The method, which has been developed in the frame of electromagnetic theory, permits application of optical methods to analysis of specular and non-specular x-ray scattering from rough gratings and mirrors using Monte Carlo calculus. The question of the closeness of results for 1D and 2D surfaces is of interest of this publication, since numerical methods for 1D surfaces are well established and efficient, and widely used for surfaces with 2D roughness [2].

2 Diffraction problem

We denote by $\mathbf{e}_x$, $\mathbf{e}_z$ and $\mathbf{e}_z$ the unit vectors of the axes of the Cartesian coordinates. The grating is a cylindrical surface whose generatrices are parallel to the z-axis and whose cross section is described by the curve Σ (Fig. 1). We suppose that Σ is not self-intersecting and d-periodic in x-direction. The grating surface is the boundary between two regions $G_\pm \times \mathbb{R} \subset \mathbb{R}^3$ which are filled with materials of constant electric permittivity $\varepsilon_\pm$ and magnetic permeability $\mu_\pm$.

We deal only with time-harmonic fields; consequently, the electric and magnetic fields are rep-

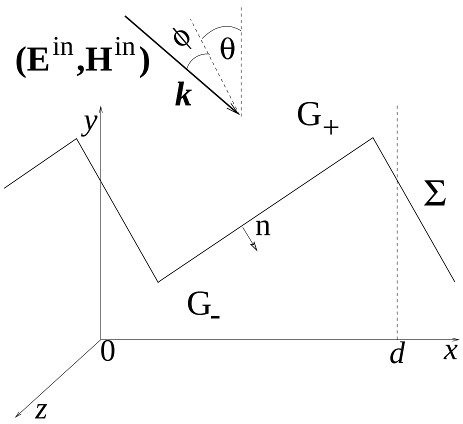

Figure 1: Schematic cross section of a grating.

resented by the complex vectors $\mathbf{E}$ and $\mathbf{H}$, with a time dependence $\exp(-i\omega t)$ taken into account. The wave vector $\mathbf{k}_+$ of the incident wave in $G_+ \times \mathbb{R}$, where $\varepsilon_+, \mu_+ > 0$, is in general not perpendicular to the grooves ($\mathbf{k}_+ \cdot \mathbf{e}_z \neq 0$). Setting $\mathbf{k}_+ = (\alpha, -\beta, \gamma)$, the surface is illuminated by a electromagnetic plane wave

$$\mathbf{E}^{in} = \mathbf{p}\ \mathrm{e}^{\,i(\alpha x - \beta y + \gamma z)}\ , \quad \mathbf{H}^{in} = \mathbf{s}\ \mathrm{e}^{\,i(\alpha x - \beta y + \gamma z)},$$

which due to the periodicity of Σ is scattered into a finite number of plane waves in $G_+ \times \mathbb{R}$ and possibly in $G_- \times \mathbb{R}$ as well. The wave vectors of these outgoing modes lie on the surface of a cone whose axis is parallel to the z-axis. This therefore is the case of conical diffraction.

The components of $\mathbf{k}_+$ satisfy the relation,

$$\beta > 0 \quad \text{and} \quad \alpha^2 + \beta^2 + \gamma^2 = \omega^2 \varepsilon_+ \mu_+\,,$$

and can be expressed through the incidence angles $|\theta|, |\phi| < \pi/2$

$$\alpha, -\beta, \gamma = \omega\sqrt{\varepsilon_+\mu_+}(\sin\theta\cos\phi, -\cos\theta\cos\phi, \sin\phi).$$

Classical diffraction corresponds to $\mathbf{k}_+ \cdot \mathbf{e}_z = 0$, whereas $\phi \neq 0$ characterizes conical diffraction.

Since the geometry is invariant with respect to any translation parallel to the z-axis, we make the ansatz for the total field

$$(\mathbf{E}, \mathbf{H})(x, y, z) = (E, H)(x, y)\ \mathrm{e}^{\,i\gamma z} \qquad (1)$$

with $E, H : \mathbb{R}^2 \to \mathbb{C}^3$. This converts the time-harmonic Maxwell equations in $\mathbb{R}^3$

$$\boldsymbol{\nabla} \times \mathbf{E} = i\omega\mu\mathbf{H} \quad \text{and} \quad \boldsymbol{\nabla} \times \mathbf{H} = -i\omega\varepsilon\mathbf{E}\,, \quad (2)$$

with piecewise constant functions $\varepsilon(x, y) = \varepsilon_\pm$, $\mu(x, y) = \mu_\pm$ for $(x, y) \in G_\pm$, into a 2D problem. This was described in [8] and analytically justified in [9]. Introducing the transverse components

$$E_T = E - E_z\mathbf{e}_z, \quad H_T = H - H_z\mathbf{e}_z,$$

representation (1) and Eqs. (2) lead to

$$\begin{aligned}(\omega^2\varepsilon\mu - \gamma^2)E_T &= i\gamma\nabla E_z + i\omega\mu\nabla \times (H_z\mathbf{e}_z),\\ (\omega^2\varepsilon\mu - \gamma^2)H_T &= i\gamma\nabla H_z - i\omega\varepsilon\nabla \times (E_z\mathbf{e}_z).\end{aligned} \qquad (3)$$

Denoting $\gamma = \omega(\varepsilon_+\mu_+)^{1/2}\sin\phi$, we introduce the piecewise constant function

$$\kappa(x, y) = \begin{cases} (\varepsilon_+\mu_+ - \varepsilon_+\mu_+\sin^2\phi)^{1/2} = \kappa_+ \in G_+ \\ (\varepsilon_-\mu_- - \varepsilon_+\mu_+\sin^2\phi)^{1/2} = \kappa_- \in G_- \end{cases} \qquad (4)$$

with the square root $z^{1/2} = r^{1/2}\exp(i\varphi/2)$ for $z = r\exp(i\varphi)$, $0 \leq \varphi < 2\pi$. As seen from (3), by the condition $\kappa \neq 0$, which will be assumed throughout, the components E_z, H_z define the electromagnetic field $(\mathbf{E}, \mathbf{H})$.

Maxwell's equations (2) imply that E_z, H_z satisfy the Helmholtz equations

$$(\Delta + \omega^2\kappa^2)\,E_z = (\Delta + \omega^2\kappa^2)\,H_z = 0 \qquad (5)$$

in $G_\pm$. The continuity of the tangential components of $\mathbf{E}$ and $\mathbf{H}$ on the surface takes the form

$$\big[(n, 0) \times E\big]_{\Sigma\times\mathbb{R}} = \big[(n, 0) \times H\big]_{\Sigma\times\mathbb{R}} = 0,$$

where $(n, 0) = (n_x, n_y, 0)$ is the normal vector on $\Sigma \times \mathbb{R}$ and $\big[(n, 0) \times E\big]_{\Sigma\times\mathbb{R}}$ denotes the jump of the function $(n, 0) \times E$ across the surface. This leads to the jump conditions for E_z, H_z across the interface Σ of the form

$$\big[E_z\big]_\Sigma = \big[H_z\big]_\Sigma = 0,$$

$$\Big[\frac{\gamma}{\omega^2\kappa^2}\partial_t H_z + \frac{\omega\varepsilon}{\omega^2\kappa^2}\,\partial_n E_z\Big]_\Sigma = \Big[\frac{\gamma}{\omega^2\kappa^2}\partial_t E_z - \frac{\omega\mu}{\omega^2\kappa^2}\,\partial_n H_z\Big]_\Sigma = 0.$$

Here $\partial_n = n_x\partial_x + n_y\partial_y$ and $\partial_t = -n_y\partial_x + n_x\partial_y$ are the normal and tangential derivatives on Σ, respectively. We introduce $B_z = (\mu_+/\varepsilon_+)^{1/2}\,H_z$ and use γ to rewrite the jump conditions in the form

$$\begin{aligned}&\big[E_z\big]_\Sigma = \big[H_z\big]_\Sigma = 0,\\ &\Big[\frac{\varepsilon\,\partial_n E_z}{\kappa^2}\Big]_\Sigma = -\varepsilon_+\sin\phi\Big[\frac{\partial_t B_z}{\kappa^2}\Big]_\Sigma,\\ &\Big[\frac{\mu\,\partial_n B_z}{\kappa^2}\Big]_\Sigma = \mu_+\sin\phi\Big[\frac{\partial_t E_z}{\kappa^2}\Big]_\Sigma.\end{aligned} \qquad (6)$$

The z-components of the incoming field

$$E_z^{in}(x,y) = p_z\, \mathrm{e}^{i(\alpha x - \beta y)}, B_z^{in}(x,y) = q_z\, \mathrm{e}^{i(\alpha x - \beta y)},$$
$$q_z = (\mu_+/\varepsilon_+)^{1/2} s_z, \qquad (7)$$

are α-quasiperiodic in x of period d, i.e. satisfy the relation

$$u(x+d,y) = \mathrm{e}^{id\alpha}\, u(x,y).$$

The periodicity of ε and μ suggests that we look for α-quasiperiodic solutions E_z, B_z. Furthermore, the diffracted fields must remain bounded at infinity, which implies the well known outgoing wave conditions

$$(E_z,B_z)(x,y) = (E_z^{in},B_z^{in}) + \sum_{n\in\mathbb{Z}} (E_n^+,B_n^+) \times \mathrm{e}^{i(\alpha_n x + \beta_n^+ y)},\ y \ge H;$$
$$(E_z,B_z)(x,y) = \sum_{n\in\mathbb{Z}} (E_n^-,B_n^-) \times \mathrm{e}^{i(\alpha_n x - \beta_n^- y)}, y \le -H, \qquad (8)$$

with unknown Rayleigh coefficients $E_n^\pm, H_n^\pm \in \mathbb{C}$, where $\Sigma \subset \{(x,y) : |y| < H\}$, and α_n, $\beta_n^\pm$ are given by

$$\alpha_n = \alpha + \frac{2\pi n}{d}, \beta_n^\pm = \sqrt{\omega^2\kappa_\pm^2 - \alpha_n^2}, 0 \le \arg\beta_n^\pm < \pi.$$

In the following it is always assumed that

$$0 \le \arg\varepsilon_-, \arg\mu_- \le \pi\,, \arg(\varepsilon_-\mu_-) < 2\pi, \qquad (9)$$

which holds for all existing optical (meta)materials. Now $0 \le \arg\kappa_-^2 < 2\pi$ and β_n^- are properly defined for all n.

Denoting the z-components of the total fields by

$$E_z = \begin{cases} u_+ + E_z^{in} \\ u_- \end{cases}, \quad B_z = \begin{cases} v_+ + B_z^{in} & \text{in } G_+ \\ v_- & \text{in } G_- \end{cases},$$

the problem (5), (6), (8) reduces now to

$$\Delta u_\pm + \omega^2\kappa_\pm^2 u_\pm = \Delta v_\pm + \omega^2\kappa_\pm^2 v_\pm = 0 \ \text{ in } \ G_\pm; \ (10)$$

$$\left.\begin{aligned} u_- &= u_+ + E_z^{in}, \frac{\varepsilon_-\partial_n u_-}{\kappa_-^2} - \frac{\varepsilon_+\partial_n(u_+ + E_z^{in})}{\kappa_+^2} \\ &= \varepsilon_+ \sin\phi\Big(\tfrac{1}{\kappa_+^2} - \tfrac{1}{\kappa_-^2}\Big)\partial_t v_-, \\ v_- &= v_+ + B_z^{in}, \frac{\mu_-\partial_n v_-}{\kappa_-^2} - \frac{\mu_+\partial_n(v_+ + B_z^{in})}{\kappa_+^2} \\ &= -\mu_+ \sin\phi\Big(\tfrac{1}{\kappa_+^2} - \tfrac{1}{\kappa_-^2}\Big)\partial_t u_-; \end{aligned}\right\}\Sigma \qquad (11)$$

$$(u_+,v_+)(x,y) = \sum_{n=-\infty}^{\infty} (E_n^+, B_n^+)\, \mathrm{e}^{i(\alpha_n x + \beta_n^+ y)},$$
$$y \ge H,$$
$$(u_-,v_-)(x,y) = \sum_{n=-\infty}^{\infty} (E_n^-, B_n^-)\, \mathrm{e}^{i(\alpha_n x - \beta_n^- y)},$$
$$y \le -H. \qquad (12)$$

A derivation of the boundary integral equations using potential operators as well as some details of the numerical implementation of Eqs. (10)–(12) can be found in Ref. 6.

3 Reflection coefficients and absorption

The reflected and transmitted diffraction orders (plane waves) of number n have the wave vectors

$$k_n^\pm = (\alpha_n,\, \beta_n^\pm,\, \gamma)$$
$$= k^\pm(\sin\theta_n^\pm \cos\phi^\pm,\, \cos\theta_n^\pm\cos\phi^\pm,\, \sin\phi^\pm),$$

with $(k^\pm)^2 - \gamma^2 \ge \alpha_n^2$. Since the z-dependence of all functions is given by $\exp(i\gamma z)$

$$\tan\theta_n^\pm = \mp\alpha_n/\beta_n^\pm = \mp\alpha_n/[(k^\pm)^2 - \gamma^2 - \alpha_n^2]^{1/2},$$
$$\phi_n^+ = \phi^+ = \phi\,, \phi_n^- = \phi^- = \arcsin(k^+\sin\phi/k^-).$$

By the convention, to ensure that $\theta_0^+ = -\theta^i$, the outgoing angles $\theta_n^\pm$ of the reflected and transmitted orders are taken from the interval $[-\pi/2\,, \pi/2]$, as well as ϕ^+ and ϕ^-.

The p and s components of diffraction order fields are defined similar to those of the incident wave (7). For a reflected or transmitted order with the wave vector $\mathbf{k}_n^\pm$ polarization angles $\delta_n^\pm$ and $\psi_n^\pm$ are determined using the scalar products $(\mathbf{E}_n^\pm, \mathbf{s}_n^\pm)$ and $(\mathbf{E}_n^\pm, \mathbf{p}_n^\pm)$

$$\delta_n^\pm = \arctan[|(\mathbf{E}_n^\pm, \mathbf{s}_n^\pm)|/|(\mathbf{E}_n^\pm, \mathbf{p}_n^\pm)|],$$
$$\psi_n^\pm = -\arg[(\mathbf{E}_n^\pm, \mathbf{s}_n^\pm)/(\mathbf{E}_n^\pm, \mathbf{p}_n^\pm)].$$

The efficiency of a diffracted order represents the proportion of power radiated in each order. Defining the power as the flux of the Pointing vector modulus $|\mathbf{P}^{in}| = \mathrm{Re}\,(\mathbf{E}^{in} \times \overline{\mathbf{H}^{in}})/2$ ($\overline{U}$ denotes the complex conjugate of U) through a normalized rectangle parallel to the (x,z)-plane, the ratio of the power of a reflected or transmitted propagating order to that of the incident wave gives the conical diffraction efficiency $\eta_n^\pm$ of this order in the simple form:

$$\eta_n^\pm = (\beta_n^\pm/\beta)\big(|(\mathbf{E}_n^\pm, \mathbf{s}_n^\pm)|^2 + |(\mathbf{E}_n^\pm, \mathbf{p}_n^\pm)|^2\big). \qquad (13)$$

If $\operatorname{Im} k^- > 0$ then there are no transmitted orders. Thus the usual law of the energy conservation, i.e. the sum of the efficiencies of all reflected and transmitted orders should be equal to the power of the incident wave, does not hold here. Instead, some part of the power is absorbed in the substrate. If the grating is absorbing, then conservation of energy is expressed by a criterion

$$R + A = \sum_{\beta_n^+ > 0} \eta_n^+ + A = 1, \qquad (14)$$

where R is the sum of the reflection order efficiencies and A is the absorption in the single-boundary off-plane problem that can be computed from integrals of the solution of the partial differential formulation of conical diffraction which is derived applying Green's formulae [6]:

$$A = \frac{(\kappa^+)^2}{\beta} \operatorname{Im}\Bigg[\frac{1}{(\kappa^-)^2}\bigg(\frac{\varepsilon^-}{\varepsilon^+}\int_\Gamma \partial_n E_z\,\overline{E_z} + \frac{\mu^-}{\mu^+}\int_\Gamma \partial_n B_z\,\overline{B_z} + 2\sin\phi\operatorname{Re}\int_\Gamma E_z\,\partial_t\overline{B_z}\bigg)\Bigg]. \qquad (15)$$

The balance requirement of Eq. (14) is one of the most important accuracy criteria based on a single computation generalized in the lossy case by the explicit computation of A from Eq. 15. The sum $R + A$ is actually the energy balance for an absorbing grating or a rough mirror in conical diffraction, and the extent to which it approaches unity is a measure of the accuracy of a calculation.

For $\lambda/d \ll 1$, the discrete order efficiencies is an approximation of the differential reflection coefficient (DRC) ζ (bistatic scattering coefficient [1]) for a continuum of scattered angles so that

$$\sum_{\beta_n^+ > 0} \eta_n^+ = \int_{-\pi/2}^{\pi/2} \zeta(\theta_n^+) d\theta_n^+. \qquad (16)$$

The general case of 2D rough surfaces may be considered in a similar way. It can be done by expressing the solution of the 3D Helmholtz equation for bi-gratings through solutions of the 2D one for classical gratings, an approach which may be resorted to in some important cases described below.

The effect of roughness on the mirror DRC can be exactly taken into account with the model in which an uneven surface is represented by a bi-grating with large periods $d_{x,z}$ in perpendicular planes, which include appropriate numbers of random asperities with correlation lengths $\xi_{x,z}$. The code analyzes a complex structure which, while being the bi-grating from a mathematical viewpoint, is actually the rough surface for $d_{x,z} \gg \xi_{x,z}$. If $\xi_{x,z} \sim \lambda$ and the number of orders is large, the continuous angular distribution of the energy reflected from randomly rough boundaries can be described by a discrete distribution η_{mn} in orders (m, n) of the bi-grating, similar to Eq. 16 for classical gratings. A study of the scattering intensity starts with obtaining statistical realizations of profile boundaries of the structure to be analyzed, after which one calculates the DRC for each realization, to end with the DRC averaged out over all realizations to obtain a mean DRC. By selecting large enough samples and numbers of sampling points, one comes eventually to properly averaged properties of the rough surface; however, this approach does not involve approximations, including averaging by the Monte Carlo method.

4 Derivation of the connection equation

A general approach to find efficiencies of bi-gratings and mean DRCs of rough 2D surfaces which permits one to use exact integral equations, rigorous (extended) boundary conditions, and radiation conditions leads to tedious calculus even in a case of perfectly conductive surfaces [10]. However, the boundary problem can be largely simplified for shallow gratings and randomly-rough surfaces if we use the Rayleigh hypothesis together with the small-amplitude perturbation technique [11–13]. Implementations of such a method, in which the reduced Rayleigh equations for reflection from such a structure are solved in the form of expansions of the amplitudes of the p- and s-polarized components of the scattered field in powers of the surface profile function through terms, up to the third order, were proposed in several papers (see Ref. 12 and references therein). In the present work the author uses results obtained in perturbative analysis only in order to derive an approximate connection rule between the efficiency of a shallow bi-grating and efficiencies of two classical gratings with grooves turned through 90 deg. The order efficiency itself of a classical grating working in conical diffraction is defined rigorously using the boundary integral equation method, as it is described above.

We will be looking for a perturbative development of the reflection operator $\mathbf{R}$ in powers of the heights $h_x^{(i)}$ and $h_z^{(j)}$ of a bi-periodic surface (either conductive or dielectric) that is the sum of the two Fourier series:

$$h(x,z) = h_x + h_z = \sum_i h_x^{(i)} \sin\bigl(2\pi x i/d_x + \tau_x^{(i)}\bigr) + \sum_j h_z^{(j)} \sin\bigl(2\pi z j/d_z + \tau_z^{(j)}\bigr). \quad (17)$$

Such a representation of $h(x,z)$ is typical for real 2D surfaces obtained, e.g., as a linear response of a photoresist to light with two separate exposures in perpendicular planes or by polishing using a linear tool. Note that the 2D Fourier transformation of $h(x,z)$ is also the sum of two 1D Fourier transforms of h_x and h_z. We assume also that the bi-grating works under arbitrary incidence and polarization states of a plane monochromatic wave, and that the respective single-periodic gratings work in conical diffraction. Suppose also for simplicity h_x and h_z are even functions that is true for many ergodic stationary processes. Replacing h_x or h_z by $-h_x$ or $-h_z$ does not change the diffraction pattern in the far-field zone. We will study the perturbative expansion of the reflected efficiency η as a function of the surface heights $(h_x^{(i)})^2$ and $(h_z^{(j)})^2$. Using the perturbative expansion of $\mathbf{R}$, the terms of η which contain an expression such as $(h_x^{(i)})^{2k}$, $(h_z^{(j)})^{2l}$ will be denoted by R_{kl}:

$$\eta \approx R_{00} + R_{01} + R_{10} + R_{11} + R_{02} + R_{20} + ...$$

Using the quasi-periodicity property of $\mathbf{R}$ [13] and Taylor expansion of scattered field amplitudes in powers of the surface profile heights (e.g, see Eq. 53 of Ref. 12), η_{mn}, η_m, and η_n can be expressed in the following form:

$$\eta_{mn} - o(h^6) = \delta_{mn} a_{00} + \sum_i a_{10}^{(i)} (h_x^{(i)})^2 + a_{20}^{(i)} (h_x^{(i)})^4 + \sum_j a_{01}^{(j)} (h_z^{(j)})^2 + a_{02}^{(j)} (h_z^{(j)})^4 + \sum_{i,j} a_{11}^{(i,j)} (h_x^{(i)} h_z^{(j)})^2, \quad (18)$$

$$\eta_m - o(h_x^6) = \delta_{m0} a_{00} + \sum_i a_{10}^{(i)} (h_x^{(i)})^2 + a_{20}^{(i)} (h_x^{(i)})^4, \quad (19)$$

$$\eta_n - o(h_z^6) = \delta_{0n} a_{00} + \sum_j a_{01}^{(j)} (h_z^{(j)})^2 + a_{02}^{(j)} (h_z^{(j)})^4, \quad (20)$$

where $\delta_{m,n}$ is the Kronecker delta.

Leaning upon physical considerations [14], we choose from Eqs. (18)–(20) one of the two possible expressions for η_{mn} through η_m and η_n:

$$\eta_{mn} - o(h^6) = \frac{\eta_m \eta_n}{a_{00}} + \sum_{i,j} \left(a_{11}^{(i,j)} - \frac{a_{m0}^{(i)} a_{0n}^{(j)}}{a_{00}} \right) \left(h_x^{(i)} h_z^{(j)} \right)^2. \quad (21)$$

Finally, using Eq. (21) one can formulate the equivalence rule:

$$\eta_{mn} = \frac{\eta_m \eta_n}{r_F} + o(h^4), \; m \vee n = 0, \; h_{x,z}/d_{x,z} < 1, \quad (22)$$

where η_m and η_n are classical grating efficiencies obtained in conical diffraction, r_F – the Fresnel factor of a surface. It is worth noting that η_m and η_n in this equivalence rule should be computed with a preservation of incidence and polarization angles of both gratings in the absolute coordinate system.

Thus the efficiency of bi-gratings can be easily expressed using Eq. (22) in terms of the product of the efficiencies of two respective classical gratings oriented in perpendicular dispersive planes and working in conical mounts at any polarization state. Equation 22 was derived in Ref. 14 for the normal incidence of linearly-polarized light on a simple-border-profile bi-grating. The considered equivalence rule is very similar to the impulse approximation result of the atomic scattering theory (see, e.g., Ref. 15) and can include multiple scattering in each direction, while always excluding cross-correlation components.

The derived connection equation is approximate and valid for shallow periodic surfaces of the type considered. However, this equivalence rule was checked successfully against various numerical examples, including non-shallow bi-gratings working at different wavelength-to-period ratios [14, 16]. It was found that it gives accurate results under the following assumptions: (a) $h_{x,z} \lesssim d_{x,z}$ and (b) $\lambda \gtrsim d_{x,z}$. However, for deterministic and non-deterministic surface profiles working in short waves some modification of these conclusions is required. As follows from the known results obtained from analytic and asymptotic expressions valid for x-rays (see, e.g., Refs. 3, 4), Eq. (16) gives high-accuracy solutions for shallow 0D (i.e. rows of atoms with displacements), 1D, and 2D surfaces if fulfilled the following conditions: (c) $\cos\chi h_{x,z} \ll d_{x,z}$ and (d) $\lambda \ll d_{x,z}$, where χ is an incidence angle on the surface. In case of x-ray-EUV ranges, refractive indices of materials are close to the vacuum refractive index and $h_{x,z}$ can be large enough, especially for grazing incidence. Thus (a) and (c) are close due to the nature of the perturbative development. However, (d) extends significantly the range of validity of Eq. (22), actually over the whole short-wave range because of the absence of optical resonances (i.e. due to plasmons, polaritons, waveguide modes, etc) in x-rays.

5 Differential reflection coefficient of x-ray Au mirror

Drawing from the above-mentioned MIM in a broad sense, we are passing on now to a study of the effect of 2D boundary topology of a continuum film on short-wave scattering intensity. We are going to demonstrate that development of mirrors requires accurate account of the film surface roughness statistics and optical mount. In this Section, the mean DRC of an Au rough mirror working at an x-ray wavelength under grazing incidence is computed using the equivalence formulae. The Au mirror has the same model of roughness in perpendicular planes which is approach closely the real conditions, to wit: in (xOy) with a Gaussian height distribution with the rms σ_x and a Gaussian autocorrelation function $C(x) = \sigma_x \exp(x^2/\xi_x^2)$; and in (yOz) with the same Gaussian height distribution and Gaussian autocorrelation function $C(z) = \sigma_z \exp(z^2/\xi_z^2)$ with $\sigma_z = \sigma_x = \sigma$ and $\xi_z = \xi_x = \xi$. Statistical surface realizations with $\sigma = 1$ nm, $\xi = 15$ nm were generated using the spectral method [1].

Figure 2 displays graphically the calculated diffuse reflectance of an Au mirror plotted vs. reflection order number (angle of scattering) in perpendicular planes for the two incident angles, $\chi = 87°$ and $\chi = 89°$, beyond the critical angle at a wavelength $\lambda = 1.54$ nm of linearly-polarized TE radiation (with the electric field vector perpendicular to the incidence plane). For the (xOy) plane χ is equal to the polar angle θ in the given diffraction problem described in Sec. 2 and for the (yOz) plane χ is equal to the azimuthal angle ϕ in the diffraction problem. The state of polarization for the first dispersive plane (classical grating) is TE, but for the second one it is TM in the given diffraction problem. To obtain the required ensemble averaging and calculation accuracy for rough surfaces, 100–200 statistical sets have to be used with 1000 points within a 1-μm interval $d_x = d_z = d$ on each. To take into account the complex structure of the rough surface and reach convergence of the results

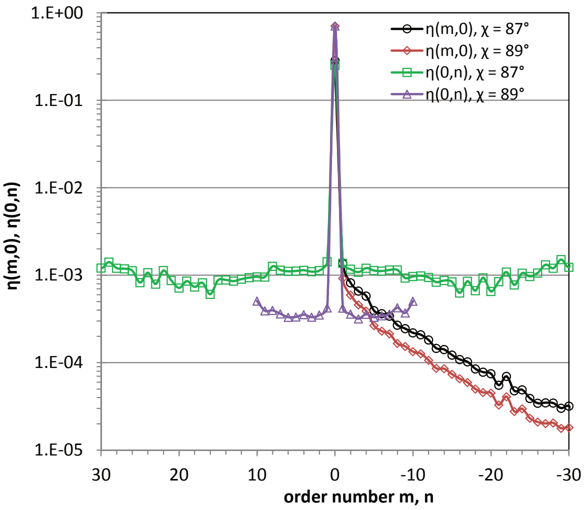

Figure 2: Scattering intensity of Au mirror in perpendicular planes in grazing-incidence x-rays.

obtained, we chose the number of collocation points $N = 2000$ in the PCGrate-SX v.6.5 code [17]. The refraction indices for Au were taken from Ref. 18.

As follows from a comparison of the curves displayed in Fig. 2, η_{0n} corresponding to the (yOz) plane is smaller than η_{m0}, which is related to the (xOy) plane, near the specular peak for $\chi = 89°$. By contrast, for $\chi = 87°$ we see that η_{0n} is larger than η_{m0} throughout the order range studied, except the specular reflection. The large difference between scattering intensities of the two identical classical gratings working in two perpendicular planes originates from the difference in grazing incidence classical and conical diffraction. In particular, η_{0n} is an approximately symmetric functions in respect to specular peaks, while η_{m0} depends only on negative order numbers. Significantly, the specular x-ray reflection coefficients are also different in perpendicular planes: $\eta_{(x)0} = 0.363$ and $\eta_{(z)0} = 0.286$ – for $\chi = 87°$ and $\eta_{(x)0} = 0.753$ and $\eta_{(z)0} = 0.740$ – for $\chi = 89°$. Note that $r_F = 0.412$ and $r_F = 0.784$ for $\chi = 87°$ and $\chi = 89°$, respectively, and the TM values of r_F are very close to the TE values for both angles of incidence (with a difference of about 0.002). Such appreciable differences between the scattering intensities of surfaces having the equal topology in perpendicular planes evidence the need of using precise roughness statistics, diffraction and polarization angles, and exact modelling tools in calculations of practical significance for a sample.

6 Conclusion

An important case of bi-periodic gratings and 2D rough surfaces may be considered in a way by expressing the solution of the 3D Helmholtz equation through solutions of the 2D general equation in conical diffraction, an approach which may be resorted to in short waves and shallow surface using the derived equivalent rule. The effect of roughness on the mirror DRC can be exactly taken into account with the model in which an uneven surface is represented by a grating with large periods in perpendicular planes, which includes a sufficient number of random asperities. Rigorous calculations revealed that diffuse x-ray scattering intensities obtained for an Au mirror with boundary profiles having the same surface statistics in perpendicular planes differ noticeably in those planes close to and far from specular peaks.

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