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Energy balance for weak formulation of diffraction by lossy anisotropic inhomogeneous gratings

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A general expression derived from Poynting's theorem reports the well-posedness of energy conservation for a weak formulation of diffraction by lossy anisotropic inhomogeneous one- and biperiodic gratings. Formulas allow direct absorption calculus with the same rigor as solutions of Maxwell's equations, i.e. via distributions employed to describe the field. Absorption integrals, valid for any rigorous method, are expressed using the near field and conductivity tensors in the volume or on the surface restricting a grating domain between uniform medias.

1 Introduction

Various optical grating properties including resonance and non-resonance anomalies, differing in their nature, can be effectively explored using structured high- and low- conductive layers, e.g.: Fano-type resonances, Brewster and Bragg conditions, Rayleigh orders, groove shape and waveguide peculiarities, anisotropic and metamaterial abilities, etc. Because of the TE and TM modes in cases for one-periodic gratings (one-gratings) in conical diffraction (Fig. 1) or biperiodic (crossed) gratings (bi-gratings) (Fig. 2) being coupled through the boundary conditions, the associated problems are more general, and gratings can act as perfect absorbers and volume- or surface-field enhancers at any incidence polarization state. Besides being physically meaningful, an accurate and fast computing of the grating absorption magnitude A is especially important for many microwave devices, in x-ray–EUV ranges, for lithography processes, in solar cell improvements and for other modern applications such as plasmonics, photonic crystals and metamaterials, where absorption plays a predominant role. Thus, a computation of A, as well as using the reciprocity theorem, is an important tool to check the quality of the numerical solution for absorbing gratings with the requirement that the sum of reflected, transmitted and total absorbed energies should be equal to the energy of the incident wave.

Another important point for analysis is that the computation of A itself is not connected with a specific rigorous method which is used for near-zone field calculus. It has not only intuitive significance but the same rigor, namely in the sense of distributions (generalized functions) and way to deduce as more simple energy conservations for perfectly conducting and lossless gratings (see, e.g., [1], Ch. 2). So, in [2] the absorption of lossy lamellar one-periodic gratings is considered for in-plane (classical) diffraction and TE/TM polarizations using the modal method. In [3] the general power balance for an anisotropic non-Hermitian one-grating is evaluated for the TM polarization (polarization wherein the electric field is in the plane of incidence) using the rigorous coupled-wave analysis. In [4] the energy conservation properties for a wave propagation through stacked gratings comprising metallic and dielectric cylinders are presented using a Green's function approach based on lattice sums to obtain the scattering matrices of each layer. In [1], Ch. 12, the generalized energy balance in the explicit form for multilayer isotropic one-gratings working in classical and

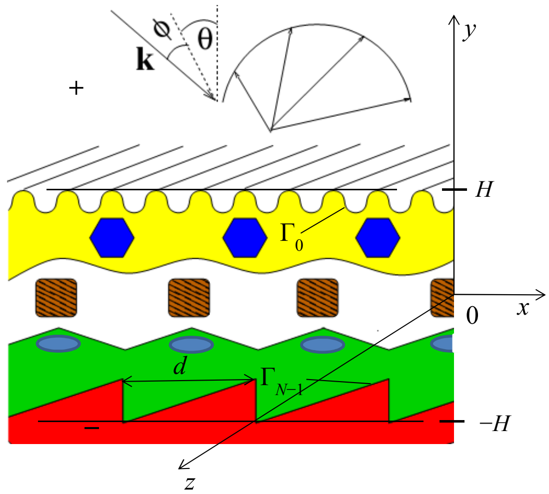

Figure 1: Schematic conical diffraction by a multilayer one-periodic grating.

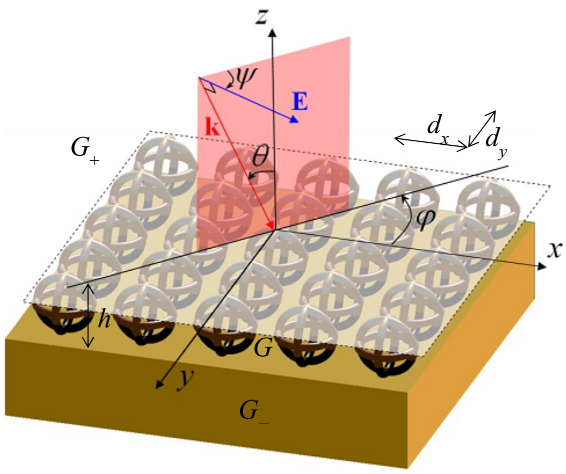

Figure 2: Schematic diffraction by a biperiodic grating.

conical diffraction is derived from the boundary integral equation theory using the absorption integrals. In [5], the energy-balance criterion described for nonlinear in-plane one-periodic gratings and rough surfaces is established in the explicit form for both polarizations and derived from Maxwell's equations. In [6], Ch. 7 the energy absorption formulae for isotropic bi-gratings is obtained using the coordinate transformation technique and boundary integral equations. In [1], Ch. 5 the global energy balance for inhomogeneous anisotropic one- and bi-gratings is presented using the finite-element method and variational formulation of the diffraction problem.

The current approach is presented for the most general case of anisotropic inhomogeneous (multilayer) bi-gratings. A derivation of explicit expressions considered for finding the absorption quantity as well as the interpretation of the results obtained for all grating types bear only on Maxwell's equations, the divergence (Gauss–Ostrogradsky) theorem and boundary conditions. Besides more generality, the present formulation is based on the rigorous mathematical foundation developed in [7–12] and related publications via variational (weak) formulations of the bi-grating diffraction problem including the existence, uniqueness and convergence of the electromagnetic field solution. These results can be used to justify the workability of a present plethora of numerical methods to solve any kind of diffraction problems rigorously. It worth noting that those methods were developed mostly by specialists in physics and optics, and, some of them, were seemingly not aware of the rapid progress in the fields of finite element methods, boundary element methods and integral equation methods made in the mathematical community since 1990. The weak formulation has the great advantage that it is applicable to very general diffraction gratings with any topology of interfaces and materials: biperiodic, inhomogeneous, anisotropic, negatively-refracted and even [13] nonlinear. In the electromagnetic literature there are various expressions for the absorption, however without a complete derivation and references to mathematical results for diffraction gratings. Thus, the energy balance generalization and computation in the explicit form (in quadratures) of A for complex one- and bi-gratings can be considered as having both academic and practical importance.

2 Diffraction problem

2.1 Problem statement

Consider the general case of vector diffraction by an arbitrary crossed grating with periods d_x and d_y directed, in general, non-orthogonally. Let a time-harmonic (with time dependence $\mathrm{e}^{-\mathrm{i}\omega t}$) electromagnetic linearly-polarized plane wave incident above $(+)$ on a bi-periodic lossy structure G bounded in $\mathbb{R}^3$ and separated by two homogeneous half-spaces $G_+ := \{z \geq 0\}$ and $G_- := \{z \leq -h\}$, $h \geq 0$ in Cartesian coordinates $(x, y, z) = \mathbf{r} \in \mathbb{R}^3$ (Fig. 2). We assume constant relative electric permittivity $\epsilon_\pm$ and constant relative magnetic permeability $\mu_\pm$ such that $\operatorname{Re}\epsilon_+ \wedge \operatorname{Re}\mu_+ > 0$, $\operatorname{Im}\epsilon_+ \wedge \operatorname{Im}\mu_+ = 0$, $\operatorname{Im}\epsilon_- \wedge \operatorname{Im}\mu_- \geq 0$. Otherwise, the relative permittivity $\hat{\epsilon}(x, y, z)$ and permeability $\hat{\mu}(x, y, z)$ functions of the grating region G are given by nonsingular 3×3 matrices with doubly periodic, complex-valued L^∞ (bounded) components. In physics, these components are usually piecewise continuous or piecewise constant functions corresponding to material refractive indices. Thus, we allow rather general anisotropic biperiodic structures including edges, corners, intersected boundaries, inclusions and also metamaterials. As it is important in the treatment of periodic problems, we restrict the consideration to one unit-cell $\Omega := \{\mathbf{r} \in Q \times \mathbb{R} : -h \leq z \leq 0\}$, for one biperiod $Q := [0, d_x) \times [0, d_y)$ and uniform regions $\Omega_\pm$ above and below Ω such that $\Omega_+ := \{\mathbf{r} \in Q \times \mathbb{R} : z > 0\}$ and $\Omega_- := \{\mathbf{r} \in Q \times \mathbb{R} : z < -h\}$ (now $\overline{\Omega}$ is a compact set).

In the physical problem the surface is illuminated by an electromagnetic plane wave with the incident wave vector $\mathbf{k}_+ = (\alpha, \beta, -\gamma)^{\mathrm{T}}$

$$u^i = (\mathbf{E}^i, \mathbf{H}^i) = (\mathbf{p}, \mathbf{s})\, \mathrm{e}^{\mathrm{i}(\alpha x + \beta y - \gamma z)}\,. \tag{1}$$

In (1) polarization vectors $\mathbf{p}$, $\mathbf{s}$ satisfy

$$\mathbf{k}_+ \cdot \mathbf{p} = \mathbf{k}_+ \cdot \mathbf{s} = \mathbf{s} \cdot \mathbf{p} = 0.$$

Due to the grating periodicity the incident wave is scattered into a finite number of plane waves in $G_+ \times \mathbb{R}$ and possibly in $G_- \times \mathbb{R}$. $|k_+| = k_v\sqrt{\epsilon_+\mu_+}$, $\epsilon_+ \neq 0 \wedge \vee \mu_+ \neq 0$, where $k_v = \frac{w}{c}$, ω is a fixed positive frequency and c is the vacuum light velocity. Note that this condition is satisfied by dielectric media with $\varepsilon_+ > 0$, $\mu_+ > 0$ as well as negative index materials, satisfying $\varepsilon_+ < 0$, $\mu_+ < 0$. The wave vector $\mathbf{k}_+$ is expressed using the incidence angles $|\theta| < \pi/2$, $|\phi| < 2\pi$ and the polarization angle $|\Psi| < \pi$:

$$\mathbf{k}_+ = k_v\nu_+(\sin\theta\cos\phi, \sin\theta\sin\phi, -\cos\theta)^T$$

and

$$\begin{aligned} p_x &= \cos\Psi\cos\theta\cos\phi - \sin\Psi\sin\phi, \\ p_y &= \cos\Psi\cos\theta\sin\phi + \sin\Psi\cos\phi, \\ p_z &= -\cos\Psi\sin\theta. \end{aligned}$$

For the upper refractive index $\nu_+ = \sqrt{\epsilon_+\mu_+}$ we determine $\gamma > 0$ if $\varepsilon_+ > 0$, $\mu_+ > 0$, whereas $\gamma < 0$ for negative index materials.

The total electromagnetic fields $u_\pm$ are given by

$$\begin{aligned} u_+ &= u^i + (\mathbf{E}_+, \mathbf{H}_+), \quad \text{in } G_+, \\ u_- &= (\mathbf{E}_-, \mathbf{H}_-), \quad \text{in } G_- \end{aligned} \tag{2}$$

and satisfy:

- quasiperiodicity by a multiplication operator $F_{\alpha,\beta}$ acting on (α, β)-quasiperiodic function $u : \mathbb{R}^3 \to \mathbb{C}$ such that

$$F_{\alpha,\beta}u(\mathbf{r}) := \mathrm{e}^{\mathrm{i}(\alpha x + \beta y)}\, u(\mathbf{r}); \tag{3}$$

- the outgoing wave conditions in the sense of Rayleigh series with coefficients $c^\pm_{n,m}$

$$\begin{aligned} u_+ - u^i &= \sum_{n,m=-\infty}^{\infty} c^+_{n,m}\, \mathrm{e}^{\mathrm{i}(\alpha^+_n x + \beta^+_m y + \gamma^+_{n,m} z)}, z \geq 0, \\ u_- &= \sum_{n,m=-\infty}^{\infty} c^-_{n,m}\, \mathrm{e}^{\mathrm{i}(\alpha^-_n x + \beta^-_m y - \gamma^-_{n,m} z)}, z \leq -h, \end{aligned} \tag{4}$$

where $\alpha_n = \alpha + 2\pi n/d_x$, $\beta_m = \beta + 2\pi m/d_y$ and $\gamma^{\pm 2}_{n,m} = k^2_\pm - \alpha^2_n - \beta^2_m$ with $\gamma^\pm_{n,m} > 0$ or $-i\gamma^\pm_{n,m} > 0$;

- boundary conditions for the tangential components of $\mathbf{E}$, $\mathbf{H}$, $\mathbf{curl}\,\mathbf{E}$ and $\mathbf{curl}\,\mathbf{H}$

$$\begin{aligned} [\mathbf{n} \times u]_{\partial\Omega_\pm} &= 0, \\ [\mathbf{n} \times \hat{\epsilon}^{-1}(\nabla \times \mathbf{H})]_{\partial\Omega_\pm} &= 0, \\ [\mathbf{n} \times \hat{\mu}^{-1}(\nabla \times \mathbf{E})]_{\partial\Omega_\pm} &= 0. \end{aligned} \tag{5}$$

The square brackets in (5) denote the jump of functions across $\partial\Omega_\pm$.

Using (4) for the field and its normal derivative representations on $\partial\Omega_\pm$ (5) can be transformed to the form of nonlocal transmission conditions (see, e.g., [9]), which satisfy

$$\begin{aligned} \partial_z u(x, y, 0) &= -T^+_{\alpha,\beta}u(x, y, 0) - 2\mathrm{i}\beta p, \\ \partial_z u(x, y, -h) &= T^-_{\alpha,\beta}u(x, y, -h), \end{aligned} \tag{6}$$

where

$$T^\pm_{\alpha,\beta}u(x, y) = \sum_{n,m=-\infty}^{\infty} -\mathrm{i}\gamma^\pm_{n,m}c^\pm_{n,m}\, \mathrm{e}^{\mathrm{i}(\alpha_n x + \beta_m y)} \tag{7}$$

with the Fourier coefficients

$$c^\pm_{n,m} = \frac{1}{d_x d_y}\int_Q u(x, y)\, \mathrm{e}^{-i(\alpha_n x + \beta_m y)}\, dxdy.$$

The pseudodifferential operators $T^\pm_{\alpha,\beta}$ acting on doubly periodic vector functions on $\mathbb{R}^2$ specify the Dirichlet-to-Neumann map. The operators $T^\pm_{\alpha,\beta}$ map the Sobolev space $H^s_p(Q)$ of doubly periodic functions defined on Q boundedly into $H^{s-1}_p(Q)$, $s \in \mathbb{R}$. The equality in (7) is valid in the sense of distributions. The space $H^s_p(Q)$ denotes the closure of smooth doubly periodic functions on $\mathbb{R}^2$ with respect to the norm

$$|c_{0,0}|^2 + \sum_{\substack{n=-\infty \\ n\neq 0}}^{\infty} \sum_{\substack{m=-\infty \\ n\neq 0}}^{\infty} |(n, m)|^{2s}|c_{n,m}|^2.$$

Note that $H^s_p(\Omega)$ denotes the restriction to Ω of all doubly periodic functions in $H^s_{loc}(\mathbb{R}^3)$ and for $u \in H^1_p(\Omega)$ the boundary values $u|_{\partial\Omega_\pm} \in H^{1/2}_p(\partial\Omega_\pm)^3$.

In the following we need vector fields $\mathbf{E}_\pm, \mathbf{H}_\pm$ of locally finite energy

$$\mathbf{E}_\pm,\ \mathbf{H}_\pm,\ \nabla \times \mathbf{E}_\pm,\ \nabla \times \mathbf{H}_\pm \in \mathbf{L}^2_{\mathrm{loc}}(\Omega^3)$$

satisfying two couples of time-harmonic Maxwell equations

$$\nabla \times \mathbf{E} = \mathrm{i}\omega\mathbf{B}, \quad \nabla \times \mathbf{H} = -\mathrm{i}\omega\mathbf{D}\,; \tag{8}$$

$$\mathbf{D} = \epsilon_v\hat{\epsilon}\mathbf{E}, \quad \mathbf{B} = \mu_v\hat{\mu}\mathbf{H}, \tag{9}$$

where ϵ_v and μ_v are vacuum constants. Thus, equations introduced in (8) and (9) together with (1)–(7) give us the full problem statement.

2.2 Energy balance for diffraction gratings

The efficiency of a diffracted or transmitted propagating mode (order) represents the proportion of power radiated in each order. Defining the power for time-harmonic electromagnetic incident fields as the flux density of the Poynting vector modulus $|\mathbf{S}^i| = \mathrm{Re}\,(\mathbf{E}^i \times \overline{\mathbf{H}^i})/2$ ($\overline{C}$ means the complex conjugate of C) through a normalized rectangle parallel to the (x, y)-plane (Fig. 2), the ratio of the power of reflected or transmitted propagating orders and of the incident wave gives the sum of diffraction efficiencies of reflected orders R or transmitted orders T. Diffraction efficiencies for the reflected and transmitted orders of any grating can easily be found from the corresponding Raleigh coefficients or boundary values, see, e.g., in [1]. If a general multilayer grating (Fig. 1) has the perfectly conducting substrate, e.g. $\nu_N = (0, \infty)$, where ν_N is a refractive index in the substrate and there is no any energy absorption in the grating layers, $\mathrm{Im}\,\hat{\nu}_j = 0$, where $\hat{\nu}_j$ are refractive index matrices, $j = 1, \ldots, N-1$; then energy conservation under unitary normalization for the incident wave is expressed by the standard energy criterion $R = 1$. If the grating is lossless, $\mathrm{Im}\,\hat{\nu}_j = 0$, $j = 0, \ldots, N$, then energy conservation is expressed by a similar energy criterion $R + T = 1$. In the most publications devoted to the theory of diffraction gratings (see, e.g., Refs. in [1]) one verifies energy conservation by calculating the real part of a surface integral over the lossless grating region for the normal component of Poynting's vector $\mathbf{S} = \mathbf{E} \times \overline{\mathbf{H}}/2$:

$$R + T - 1 = \mathrm{Re} \oint \mathbf{S}\mathbf{n}\, ds = 0. \tag{10}$$

If $\mathrm{Im}\,\hat{\nu}_j > 0$ for some $j = 1, \ldots, N$, then there is some energy absorption in grating layers or/and in the substrate. Thus, the above mentioned principle of energy conservation (the sum of efficiencies of all reflected and transmitted orders should be equal to the power of the incident wave) does not hold. In a general case,

$$A + R + T = 1, \tag{11}$$

where A is called the absorption coefficient or simply the absorption in the given diffraction problem. In the lossy case, an independently calculated quantity A is required to verify (11). In particular, the values of the field on $\partial\Omega_+$ and $\partial\Omega_-$ can give valuable information on the absorbing power ([1], Ch. 12). To find such a quantity a valid approach should be used because some arbitrariness exists in the definition of $\mathbf{S}$ as well in the calculation of the surface integral in (10) (see, e.g., in [14]). Knowledge of a directly calculated value of the absorption for a grating is a useful and self-consistent tool not only for single-computation testing the correctness and reliability of developed computer codes. In many difficult cases convergence of A has to be compared with convergence of the indirect absorption $A_i = 1 - R - T$ due to numerical differences in the concrete rigorous method to compute near- and far-zone fields (see, e.g., in [1] and [15–17]).

3 Absorption problem

3.1 Energy balance derivation

The present formulation for the energy balance and absorption coefficient of anisotropic inhomogeneous bi-gratings follows the classical line on the complex Pointing theorem applying. Suppose from [7–12] that $\mathbf{E}$, $\mathbf{H}$ are a solution of the partial differential formulation of the diffraction problem (1)–(9), the expression for the energy balance and absorption can be derived from Maxwell's equations for $\mathbf{curl}\,\mathbf{E}$ and $\mathbf{curl}\,\mathbf{H}$ in a periodic cell Ω, which has in x-direction the width d_x, in y-direction the width d_y and is bounded by planes $z = 0$, $z = h$ and contains $\partial\Omega$. From (8) and (9) one can derive after some algebra the well-known relation for the time-averaged complex field amplitudes and Poynting's vector

$$\nabla\, \mathrm{Re}\, \mathbf{S} = -(\epsilon_v \overline{\mathbf{E}} \hat{\sigma}_e \mathbf{E} + \mu_v \overline{\mathbf{H}} \hat{\sigma}_m \mathbf{H})/2, \tag{12}$$

where $\hat{\sigma}_e = \mathrm{i}\omega\epsilon_v(\hat{\epsilon} - \tilde{\epsilon})/2$ and $\hat{\sigma}_m = \mathrm{i}\omega\mu_v(\hat{\mu} - \tilde{\mu})/2$ are relative electric and magnetic, resp., conductivity tensors and $\tilde{\epsilon}$ and $\tilde{\mu}$ are hermitian conjugates to tensors $\hat{\epsilon}$ and $\hat{\mu}$ (e.g. obtained by a matrix transposition and complex conjugations of matrix elements), resp. Then we integrate (12) over the volume Ω. Making the use of the Green–Ostrogradsky theorem for the left term and integration by parts lead to

$$\mathrm{Re} \int_{\partial\Omega_+} \mathbf{S}^i \mathbf{n}\, ds + \mathrm{Re} \int_{\partial\Omega_+} \mathbf{S}\mathbf{n}\, ds + \mathrm{Re} \int_{\partial\Omega_-} \mathbf{S}\mathbf{n}\, ds + \frac{1}{2} \left[\int_{\Omega} \epsilon_v \overline{\mathbf{E}} \hat{\sigma}_e \mathbf{E} + \mu_v \overline{\mathbf{H}} \hat{\sigma}_m \mathbf{H} dv \right] = 0, \tag{13}$$

where $\mathbf{n}$ refers to the exterior unit vector normal to the surfaces $\partial\Omega_\pm$ enclosing Ω. Taking into account

(4), (6), (10), the equality (13) can be transformed to

$$\tilde{I} - \tilde{R} - \tilde{T} = \frac{1}{2}\int_{\Omega}\big(\epsilon_v \overline{\mathbf{E}}\hat{\sigma}_e \mathbf{E} + \mu_v \overline{\mathbf{H}}\hat{\sigma}_m \mathbf{H}\big)dv, \quad (14)$$

where $\tilde{I}$, $\tilde{R}$ and $\tilde{T}$ are unnormalized incident, reflected and transmitted power z-components, resp. The first three terms in (13) are real quantities and the fourth term should be also real. So, we come finally to the energy balance

$$\tilde{A} + \tilde{R} + \tilde{T} = \tilde{I} \quad (15)$$

with the unnormalized absorption coefficient

$$\tilde{A} = \frac{1}{2}\,\mathrm{Im}\int_{\Omega}\big(\epsilon_v \overline{\mathbf{E}}\hat{\sigma}_e \mathbf{E} + \mu_v \overline{\mathbf{H}}\hat{\sigma}_m \mathbf{H}\big)dv, \quad (16)$$

valid for any grating and rigorous method in use.

3.2 Weak formulation results

Maxwell equations been valid for generalized functions, (16) is valid in the same sense. The general existence, uniqueness and stability (continuity) of a solution for $\tilde{A}$ formally results immediately from the strong ellipticity concept via the variational formulations for $\mathbf{E}$ and $\mathbf{H}$ derived from the mentioned above rigorous mathematical studies [7–12]. As a result, the Poynting vector and its divergence are continuous on $\partial\Omega_{\pm}$. Hence, the right part of (12) is also continuous.

The basic idea of a variational approach is to establish a coercitivity for the bilinear form of the variational formulation in the energy space and then apply the Lax–Milgram lemma and the Fredholm alternative [18]. The time harmonic Maxwell equations are transformed to an equivalent strongly elliptic variational problem for the electric or/and magnetic field in a bounded biperiodic cell with nonlocal boundary conditions using, e.g, Galerkin's formulation (see in [1], Ch. 5). This guarantees the existence of quasiperiodic electric (resp., magnetic) fields solving Maxwell's equations and justifies the discretization of the biperiodic diffraction problem with standard finite elements.

It was shown that the grating variational problem is solvable for all frequencies and directions of the incident wave. The solutions for $\mathbf{E}$ and $\mathbf{H}$ are unique except for a discrete sequence of frequencies accumulating at infinity. If the structure contains absorbing materials and the permittivity tensors are piecewise analytic, as it is in most cases, then the diffraction problem is uniquely solvable for all frequencies [12].

4 Absorption coefficients

4.1 Absorption coefficients of bi-gratings

Equation (16) determines the absorption power in a grating volume. In diffraction efficiency and absorption calculus the respective magnitude should be normalized to the power of the incident wave. In our case it should be the time-averaged Poynting vector z-component of the incident flux density within a rectangle surface of area $d_x d_y$ parallel to the (x, y)-plane and having the upper medium impedance:

$$\tilde{I} = \Big|\mathrm{Re}\int \mathbf{S}^i \mathbf{z}\, dxdy\Big|.$$

Using the incident wave (1) with the electric polarization vector of the unitary amplitude, $|\mathbf{p}| = 1$, and boundary conditions (6) one can calculate this integral easily in the explicit form

$$\tilde{I} = d_x d_y \cos\theta \sqrt{\epsilon_+/\mu_+})/(2Z_v). \quad (17)$$

where $Z_v = \sqrt{\mu_v/\epsilon_v}$ is the vacuum impedance. Using (17) and (16) the general normalized absorption coefficient $A = \tilde{A}/\tilde{I}$ of a bi-grating is introduced as

$$A_2 = \frac{\sqrt{\mu_+/\epsilon_+}}{2d_x d_y \cos\theta}\,\mathrm{Im}\int_{\Omega}\big(\overline{\mathbf{E}}\hat{\sigma}_e \mathbf{E} + Z_v^2 \overline{\mathbf{H}}\hat{\sigma}_m \mathbf{H}\big)dv. \quad (18)$$

Equation (18) represents the main result for the absorption of any bi-grating described above and is used in the normalized energy balance of (11) to test numerical codes. It is valid for any rigorous electromagnetic method that can derive local values of $\mathbf{E}$ and $\mathbf{H}$ in the volume of one grating period. Such a directly calculated absorption can be (and should be) compared to the indirect value of A_i to check the accuracy of results. However, for some rigorous approaches like boundary integral equation methods, boundary element methods, methods of fictitious sources, surface integrals are much more preferable to calculate. For such numerical methods direct calculus of A using a surface (or contour, for one-gratings) integral for the Poynting vector component over the closed grating region can be used. It reads by (13) and (17) as

$$A_2 = \frac{Z_v\sqrt{\mu_+/\epsilon_+}}{2d_x d_y \cos\theta}\,\mathrm{Re}\int_{\partial\Omega} \mathbf{E} \times \overline{\mathbf{H}}\mathbf{n}\, ds. \quad (19)$$

and describes the same as in (18), i.e. the Joule effect losses density of the absorbing grating. The advantage of (18) in compare with (19) might be using only one of two solutions $\mathbf{E}$ or $\mathbf{H}$ of the diffraction problem for some materials. For example, for a grating medium with the real scalar magnetic permeability $\hat{\mu} = \tilde{\mu} = \mu$, $\hat{\sigma}_m = 0$ and (18) reads

$$A_2 = \frac{\sqrt{\mu_+/\epsilon_+}}{2d_x d_y \cos\theta} \operatorname{Im} \int_\Omega \overline{\mathbf{E}}\hat{\sigma}_e \mathbf{E} dv. \tag{20}$$

For so called z-anisotropic kinds of materials, $-\hat{\epsilon} = \tilde{\epsilon}$, and for grating regions with the real scalar μ (20) transforms to the known formulae which is used with the finite element and rigorous coupled-wave methods [see, e.g., [1], Ch. 5, [19])

$$A_2 = \frac{\sqrt{\mu_+/\epsilon_+}}{d_x d_y \cos\theta} \int_\Omega \operatorname{Im} \hat{\epsilon} |\mathbf{E}|^2 dv. \tag{21}$$

4.2 Absorption coefficients of one-gratings

For one-gratings very similar results for the absorption A_1 can be obtained on the basis of the respective weak formulation or other mathematical proofs (see in [18]) taking into account that the field does not vary in one coordinate. The volume integral in (18) should be exchanged to the surface one for a rectangle surface $\partial\Omega'$ of area $d_x \cdot h$ (Fig. 2) and with the new normalization for the incident power

$$A_1 = \frac{\sqrt{\mu_+/\epsilon_+}}{2d_x \cos\theta} \operatorname{Im} \int_{\partial\Omega'} \big(\overline{\mathbf{E}}\hat{\sigma}_e \mathbf{E} + Z_v^2 \overline{\mathbf{H}}\hat{\sigma}_m \mathbf{H}\big) ds. \tag{22}$$

Applying to (22) the same restrictions as to (21) we derive for one-gratings

$$A_1 = \frac{\sqrt{\mu_+/\epsilon_+}}{d_x \cos\theta} \int_{\partial\Omega} \operatorname{Im} \hat{\epsilon} |\mathbf{E}|^2 ds. \tag{23}$$

In [1], Ch. 12, a derivation of the energy balance and A_1 for isotropic one-gratings working in classical or conical (azimuthal angle $\phi \neq 0$) diffraction (Fig. 1) is based on computations of the respective contour integrals by values of the fields $E(x, y, z) = E(x, y)\,\mathrm{e}^{\mathrm{i}\gamma z}$ and $U(x, y, z) = Z_v H(x, y)\,\mathrm{e}^{\mathrm{i}\gamma z}$, $\gamma = \omega\sqrt{\epsilon_+\mu_+}\sin\phi$ and their normal (∂_n) and tangential (∂_t) derivatives on a grating boundary Γ:

$$A_1 = \frac{1}{\beta} \operatorname{Im}\Big[\frac{\kappa_+^2}{\kappa_-^2}\Big(\frac{\varepsilon_-}{\varepsilon_v}\int_\Gamma \partial_n^- E_z \overline{E_z} + \frac{\mu_-}{\mu_v}\int_\Gamma \partial_n^- U_z \overline{U_z} + \sqrt{\frac{\epsilon_+\mu_+}{\epsilon_v\mu_v}}\, 2\sin\phi \operatorname{Re}\int_\Gamma E_z \partial_t^- \overline{U_z}\Big)\Big], \tag{24}$$

where $\kappa_\pm = \epsilon_\pm\mu_\pm - \epsilon_+\mu_+ \sin\phi$ in the upper (+) and lower (−) mediums, $\epsilon_\pm$ and $\mu_\pm$ are electric permittivities and magnetic permeabilities, resp., β is the wave vector y-component, $\mathbf{n}$ is the outward unit vector of the normal and arc length integration is performed assuming $d = 1$ along one period Γ of the cut of the boundary by the $z = 0$ plane.

For multilayer gratings A_1 is similarly calculated as the difference between the energy flux densities that cross the upper, Γ_0, and the lower, Γ_{N-1}, boundaries of the multilayer structure through cells $\Omega_{\pm H}$ bounded by planes $x = 0$, $x = d$, $z = 0$, $z = 1$, $y = \pm H$ and contained Γ_0 or Γ_{N-1}:

$$A_1 = \frac{1}{\beta} \operatorname{Im}\Big[\int_{\Gamma_0} \Big(\frac{\epsilon_+}{\epsilon_v}\partial_n^+ E_z \overline{E_z} + \frac{\mu_+}{\mu_v}\partial_n^+ U_z \overline{U_z}\Big) - \frac{\kappa_+^2}{\kappa_-^2}\int_{\Gamma_{N-1}} \Big(\frac{\varepsilon_-}{\varepsilon_v}\partial_n^- E_z \overline{E_z} + \frac{\mu_-}{\mu_v}\partial_n^- U_z \overline{U_z}\Big)\Big], \tag{25}$$

where $\mathbf{n}_0$ and $\mathbf{n}_{N-1}$ are unit vectors of the normal, which are interior to the regions under study.

From the detailed mathematical analysis of the conical diffraction solution using boundary integral equations the Fredholmness of operators V^+ and V^- has been established with such basic properties:

1. The integral equations are equivalent to the Helmholtz system if the operators V^+ and V^- are invertible.
2. If the profile Γ has no corners, then the problem is solvable if $\varepsilon_- + \varepsilon_+ \neq 0$ and $\mu_- + \mu_+ \neq 0$.
3. If the profile Γ has corners, then the problem is solvable if $\varepsilon_-/\varepsilon_+$ and $\mu_-/\mu_+ \notin [-\rho, -1/\rho]$ for some $\rho > 1$, depending on the angles at these corners.
4. The solution of the problem is unique if $\operatorname{Im}\varepsilon_- \geq 0$ and $\operatorname{Im}\mu_- \geq 0$ with $\operatorname{Im}(\varepsilon_- + \mu_-) > 0$.

Conclusion

A generalization of the energy balance, presented for lossy anisotropic inhomogeneous one- and biperiodic gratings, is based on a diffraction problem variational formulation and does not depend on a rigorous method chosen to solve Maxwell's equations. This guarantees the existence, uniqueness and solvability under computations of the respective absorption integrals. It can be done by the derived general formulas via known near-zone field values and conductivity tensors, either in the grating volume or on its boundary. Thus, the present energy balance derivation for very general absorbing gratings can be considered as universal and useful as well-known energy conservations for perfectly conducting and lossless gratings. The proposed approach can be extended also to non-linear gratings and randomly rough surfaces that is a matter of future publications.

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