Coherent and incoherent phenomena in anisotropic periodic gratings

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***Abstract*—This paper deals with modeling of incoherent and partialy coherent effects in structures with lateral periodicity based on scattering matrix formalism. The recurrent formulas are applied in matrix form to describe structures consisting of general anisotropic materials. Incoherent wave summation is presented in the form of infinite geometric series and generalized Mueller matrix calculus descibing complete polarimetric response including depolarization phenomena. This method can be combined with any of the existing coherent methods of modeling periodic structures and it offers significantly faster computational performance than partially coherent/incoherent methods based on averaging. The general approach is demonstrated on phenomena emerging from the complex interaction between diffraction grating and thick substrate and the models are compared with experimental spectroscopic data.**

***Index Terms*—periodic structure, incoherent summation, Rigorous Coupled Wave Analysis, Mueller matrix.**

I. Introduction

Majority of widely applied rigorous methods for precise modeling of electromagnetic fields in periodic structures, like Rigorous Coupled-Wave Analysis (RCWA) [1], Finite-Difference Time-Domain method (FDTD) [2], Finite Element Method (FEM) [3], Plane-Wave Admittance Method (PWAM) [4] are based only on illumination by coherent light. In such coherent models interference phenomena occur for arbitrary long optical path difference. This approach is sufficient for many applications, but is not enough in specific areas, as the presence of incoherent or partialy coherent light can suppress or attenuate interference oscillations and drastically change the properties of investigated systems.

In spectroscopic or ellipsometric experimental measurements and many cases of practical interest, the incoherency can have multiple origins: the presence of thick transparent substrate, as the thickness of substrate usually exceeds the coherence length of the light source; by inhomogenity in the thickness of the measured sample over the beam spot; span of incident angles; or the finite spectral bandwidth of the monochromator.

In this paper, we introduce a new method based on Mueller matrix formalism for modeling of incoherent effects in systems containing periodic structures consiting of materials with arbitrary anisotropy. The proposed method combines the scattering matrix (S-matrix) approach, as a way of describing the optical response of a coherent system, with a Partial Wave Summation Method [5], [7] and Mueller matrix formalism widely used in optical community [6]. As our approach is a matrix method based on Mueller matrix formalism, also depolarization of light by the structure is described and no statistical averaging is needed, which increases the numerical efficiency of the algorithm especially for complex structures. The method also enable deeper understanding and physical insight of a complex wave propagation in periodic systems.

II. Matrix description of polarized light

Coherent propagation can be effectively described using the 2×2 amplitude-based Jones polarization matrix $\mathbf{R}$, which consists of the aplitude reflection coefficiets r_{ss}, r_{sp}, r_{ps}, and r_{pp}. The lower indexes correspond to incident and refelected polarizations. To describe incoherent effects properly and to avoid spurious interferences, intensity based statistical quantities like Mueller matrices, instead of amplitudes need to be summed. The 4×4 intensity-based Mueller matrices describing the interaction with the sample can be obtained from the amplitude based Jones matrices by the following transformatios $\mathcal{R} = \mathbf{A}\left(\mathbf{R} \otimes \mathbf{R}^*\right)\mathbf{A^{-1}}$, where $\otimes$ denotes the Kronecker product and $\mathbf{A}$ is a lienar transformation matrix [5].

The presence of the grating periodicity Λ introduces diffraction behavior. The effective propagation constant of the n-th mode in one-dimensional case takes the form:

$$N_{y,n} = N_{y,0} + n\frac{\lambda}{\Lambda}, \tag{1}$$

where $N_{y,0}$ describes incident wave, λ denotes the light wavelength.

III. Incoherent partial wave summation

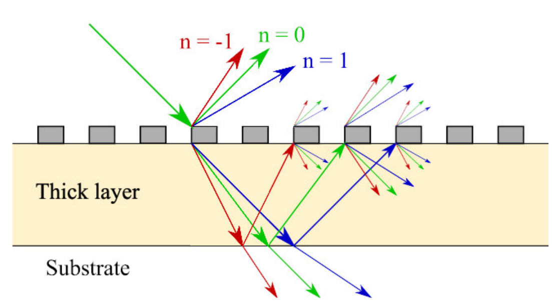


Fig. 1. Partial wave summation in system with lateral periodicity

The incident light upon hitting the first interface is partially reflected and partially transmitted, as seen in Fig. 1. The transmitted waves then propagate through the thick layer, where they can be absorbed, but the phase information is lost. At the second interface the waves are again partially reflected and transmitted. This interaction can be described in the form of matrix sum and leads to a convergent infinite series with finite sum known as Airy summation. This approach leads to partial summation formulas for reflection and transmission Mueller matrices of a thick layer [5], [7]:

$$\mathcal{T} = \mathcal{T}^{(1)}\mathcal{P}\left(\mathcal{I} - \widetilde{\mathcal{R}}^{(0)}\widetilde{\mathcal{P}}\mathcal{R}^{(1)}\mathcal{P}\right)^{-1}\mathcal{T}^{(0)}, \tag{2}$$

$$\mathcal{R} = \mathcal{R}^{(0)} + \widetilde{\mathcal{T}}^{(0)}\widetilde{\mathcal{P}}\mathcal{R}^{(1)}\mathcal{P}\left(\mathcal{I} - \widetilde{\mathcal{R}}^{(0)}\widetilde{\mathcal{P}}\mathcal{R}^{(1)}\mathcal{P}\right)^{-1}\mathcal{T}^{(0)} \tag{3}$$

where $\mathcal{I}$ is the identity matrix and $\mathcal{P}$ is the propagation matrix.

Such a simple procedure can be generalized for layers with lateral periodicity and the size of matrices increases significantly according to $([4(2N+1)]^2 \times [4(2N+1)]^2)$ and, the interactions between various diffraction orders need to be accounted properly (for implementation details see Supplement of Ref. [7]).

For partial coherent case, the interference effects are suprressed partialy and the Mueller matrix is expressed in the form

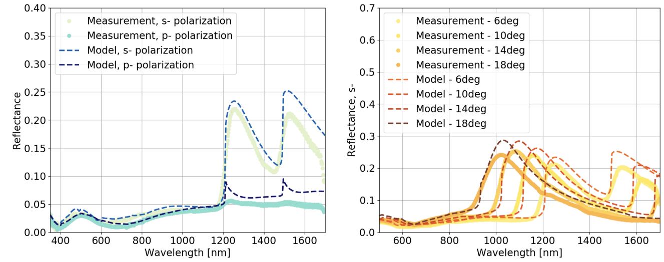
$$\begin{aligned}\mathcal{T} &= \mathcal{T}^{(12)}\mathcal{P}\,(\mathcal{E}-\mathcal{Q})^{-1}\left\{[\mathcal{E}-\gamma(\tau)\,(\mathbf{E}\otimes\mathbf{Q}^{*})]^{-1} + \right.\\ &\left.[\mathcal{E}-\gamma(\tau)\,(\mathbf{Q}\otimes\mathbf{E})]^{-1} - \mathcal{E}\right\}\mathcal{T}^{(01)},\end{aligned} \tag{4}$$

where $\mathcal{Q} = \widetilde{\mathcal{R}}^{(10)}\,\widetilde{\mathcal{P}}\,\mathcal{R}^{(12)}\,\mathcal{P}$, $\mathbf{Q} = \widetilde{\mathbf{R}}^{(10)}\,\widetilde{\mathbf{P}}\,\mathbf{R}^{(12)}\,\mathbf{P}$ and $\mathcal{E}$ is the 4×4 identity matrix and $\mathbf{E}$ is the 2×2 identity matrix. Here $\gamma(\tau)$ is the degree of mutual coherence for quasimonochromatic light of Lorentz spectral shape. Note that for $\gamma=0$ and $\gamma=1$ the formula (4) is reduced to (2) and to coherent case $\mathbf{T} = \mathbf{T}^{(12)}\mathbf{P}\,(\mathbf{E}-\mathbf{Q})^{-1}\,\mathbf{T}^{(01)}$. respectively. Reflection matrix $\mathcal{R}$ can be obtained in similar form.

IV. Generalization to Systems with Lateral Periodicity

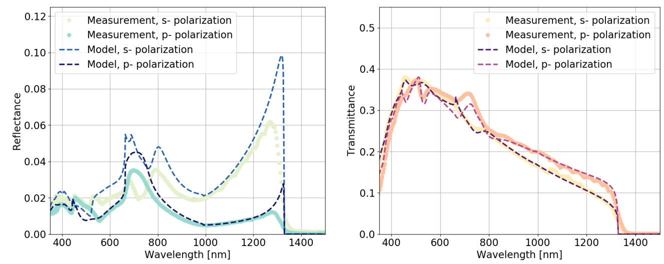
To verify applicability of our approach to structures of practical interest, the models were compared with experimental measurements on flexible diffractive components. The sample consisted of a 530 nm thick lamellar grating with the period of 1350 nm printed in a 80 μm thick polymer substrate. The s- and p- reflectance and transmittance of the zero and first diffraction orders were measured in wavelength range from 350 to 1700 nm on the Cary 7000 Spectrophotometer with Universal Measurement Accessory.

The data shows interesting effect of increased reflection with two peaks around 1250 and 1500 nm originating from the interaction of grating with the substrate, that can not be explained by models with infinite substrate.



(a) (b)

Fig. 2. Comparison of measured and modelled data. a) s- and p-specular reflectance for the incidence angle $\varphi = 6°$. b) s- reflectance for different incidence angles.



(a) (b)

Fig. 3. Comparison of measured and modelled data. a) s- and p-reflectance of first-order diffracted wave for normal incidence. b) s- and p-transmittance of first-order diffracted wave.

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