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Occurrence and significance of evanescent fields in structured samples

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ABSTRACT

Spectroscopic ellipsometry is currently widely used to describe the polarimetric response of structured media. The conceptional shortcomings of the commonly used Fresnel approach to predict and simulate ellipsometric data of structured media is discussed using numerical solutions of Maxwell's equations. Fresnel's relations and Snell's law are, strictly speaking, not valid anymore. We explain via simple physical models the effects occurring at non-horizontal interfaces between different materials. At such interfaces, evanescent fields occur and modify the still well defined complex reflectivities for s- and p-polarization. When the field vector projected on the sample surface is neither parallel nor perpendicular to the interface, the fields for s- and p-polarization couple and cross-polarization arises from the different spatial behavior of the evanescent fields.

1. Introduction

Spectroscopic ellipsometry (SE) is increasingly used to describe the polarimetric response of structured media, especially for critical dimension analysis [1]. It proves highly useful as a tool for nondestructive analysis, although the evaluation relies heavily on numerical techniques for solving Maxwell equations with e.g. finite elements (FEM, e.g. Ref. [2]) or, for periodic sample structures, with Fourier based techniques such as rigorous coupled wave analysis (RCWA). Even though the mathematics of solving Maxwell's equations numerically is well established, the understanding of physical processes arising at structured samples is not well understood. In purely stratified layers with in-plane homogeneity, the well known Fresnel relations are used to describe the polarimetric response. For non-horizontal material interfaces – grating structures and roughness also constitute non-horizontal interfaces between two materials – no general analytic solutions exist. In order to discuss the effects of these interfaces, we start with Maxwell's equations and their continuity requirements.

Optics of materials is generally described by the macroscopic Maxwell equations, in their differential form:

$$\nabla \cdot \vec{D}\left(\vec{r},t\right) = \rho\left(\vec{r},t\right) \quad \nabla \times \vec{E}\left(\vec{r},t\right) = -\partial\vec{B}\left(\vec{r},t\right)/\partial t$$
$$\nabla \cdot \vec{B}\left(\vec{r},t\right) = 0 \quad \nabla \times \vec{H}\left(\vec{r},t\right) = \partial\vec{D}\left(\vec{r},t\right)/\partial t + \vec{J}\left(\vec{r},t\right)$$

where $\vec{E}$ represents the *macroscopic* electric field, $\vec{D}$ the *macroscopic* electric displacement field, $\vec{H}$ the magnetic field strength and $\vec{B}$ the magnetization in SI representation. The behavior can be altered by the presence of free charges and current densities, ρ and $\vec{J}$ respectively. At optical frequencies however, such effects are usually considered negligible. We emphasize *macroscopic*, because these macroscopic electric fields are obtained by averaging over rather many unit cells of the solid and they are related to the wavelength of the incoming light. In addition, constitutive relations are needed to relate the fields $\vec{D}$ and $\vec{E}$. The magnetic terms are related by $\vec{B} = \mu_0\mu(\omega)\vec{H}$ with the relative permeability $\mu(\omega) = 1$ in the optical regime. Using a linear and local constitutive relation $\vec{D} = \varepsilon_0\varepsilon(\omega)\vec{E}$, it is possible to decouple the fields by rewriting the Maxwell equations into Helmholtz equations considering the harmonic solutions. However, if there are two different materials present, the permittivity formally becomes position dependent: $\varepsilon = \varepsilon(\omega, \vec{r})$. This immediately shows that a simple plane wave cannot be a solution anymore. This in-plane position dependence also implies the invalidity of Snell's and Fresnel's law, which derivations require in-plane homogeneity.

If we employ constitutive relations at an interface between two media (e.g. Au and Si) we make errors from a quantum mechanical point of view: within a small region of ~ 5–10 atomic layers on both sides of the interface, the permittivity also depends on the distance to the interface (i.e. $\varepsilon(\omega, \vec{r}, \vec{r}')$) but, beyond these 5–10 layers, the material will again be homogeneous and isotropic in the macroscopic Maxwell relations. However, this interface or surface effects are negligible by replacing (in a very good approximation) the "true", but unknown position dependent permittivity by the "bulk" permittivity for solving the Maxwell equations.

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Although $\varepsilon(\omega, \vec{r})$ is discontinuous at these interfaces, certain components of the macroscopic Maxwell equations have to be continuous *at all points in space, including at such interfaces*; these boundary conditions are derived from the integral formulation of Maxwell's equations:

$$\vec{E}_{\parallel}^{(1)} = \vec{E}_{\parallel}^{(2)} \quad \vec{D}_{\perp}^{(1)} = \vec{D}_{\perp}^{(2)}$$
$$\vec{H}_{\parallel}^{(1)} = \vec{H}_{\parallel}^{(2)} \quad \vec{B}_{\perp}^{(1)} = \vec{B}_{\perp}^{(2)}$$

Fresnel equations and Snell's laws can be derived only for planar and in-plane homogeneous samples. One has to keep in mind that their derivation uses the assumption of a planar interface separating two in-plane homogeneous isotropic bulk regions. The term "in-plane homogeneity" refers here to the condition that an arbitrary translation along the surface does not change the physics. In other words, the Fresnel equations rely on translational invariance along the surface and therefore are only correct for homogeneous samples. As a side remark, we mention that although materials are structured by atoms, homogenization works well as atomic distances a are much smaller $a \ll \lambda$ compared to the wavelength in the material – in the order of $\sim 10^{-3}$ [3].

Therefore, the Fresnel approach cannot be used to describe inhomogeneous samples (e.g. structured planar or etched Si gratings) with in-plane position dependent dielectric function such as diffractive structures usually described by a (stepwise) $\varepsilon(\vec{r})$.

Similarly, great care must be taken when applying Snell's law and the law of reflection, and the continuity of the tangential component of the wave vector $\vec{k}_{\parallel}$. The direction of the reflected/transmitted light of a grating cannot be described by a single wave vector $\vec{k}$ any more; there are now infinitely many $\vec{k}_r$, $\vec{k}_t$ vectors reflected/transmitted, some of them propagating, some of them evanescent. Snell's law is equivalent to the requirement of continuity of $\vec{k}_{\parallel}$. Because Snell's law fails in structured samples, this often used condition on the continuity of $\vec{k}_{\parallel}$ is also void. What remains valid however, are the continuity relations of the respective components of the $\vec{D}$ and $\vec{E}$ fields. In this paper, we aim to provide throughout a few examples a physical interpretation – supported by a simple simulation setup – of what happens at interfaces in structured surfaces and why care must be taken when using the effective medium approach in ellipsometric modeling of inhomogeneous, structured samples.

2. Methods

We use the rigorous coupled wave analysis (RCWA) semi-analytical method [4–6] in conical diffraction [7] implemented in *Reticolo* [8] for calculating the reflection coefficients, intensity patterns and field distribution [9]. RCWA has a worse convergence than finite elements for most problems; however, it yields a good physical picture for explaining phenomena occurring at vertical interfaces, because it is compatible with the familiar "diffraction effects" picture.

The following one dimensional setup is considered (see Fig. 1): a silicon substrate is periodically structured on its surface with 200 nm deep trenches filled with gold in the x direction and infinitely extended in the y direction. The structure is illuminated by a harmonic plane wave with given polarization at a 45° polar angle denoted by θ. The azimuthal angle φ is varied in the different simulations. Setups for which the grating vector is not contained in the plane of incidence are termed conical diffraction. Gold has a penetration depth in the order of 20 nm at the selected wavelength $\lambda_0 = 500$ nm, therefore the contributions of the reflections arising at the lower gold-silicon horizontal interface are small. Similarly, the width of the trenches as well as the periodic length are chosen

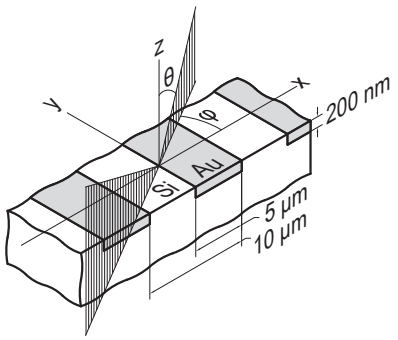

Fig. 1. Simulation setup; a 1-dimensional silicon/gold grating on silicon substrate is under plane wave illumination in conical mounting.

wide enough (10 µm) to strongly suppress the effect of neighboring structures on the total field.

Because the periodic length is large compared to the wavelength, a large number of harmonics is necessary for the solution to converge. This being said, the simple nature of the structure and the use of symmetries allows a rather fast computation of those. Simulations were performed using harmonics in the [−800;800] range. As a first test criterion, we use the convergence of the reflected intensity when increasing the number of harmonics. With the selected number of harmonics, the relative difference $\eta(n) = (\mathrm{eff}[n] - \mathrm{eff}[n-1])/\mathrm{eff}[n-1]$ is smaller than 10^{-6} for both the s- and p-polarizations, p-being known to converge slower. Here, $n = 800$ is the limit to the number of harmonics and eff[n] the related efficiency. The relative difference for each reflected diffracted order are also below 10^{-6}. For transparent samples, one can use the energy conservation that the sum of transmitted and reflected energies equals the incident energy.

Firstly, we have to mention that any Maxwell solver calculates the *total* field distribution. In ellipsometry we are used to thinking of superposing incident and reflected fields and in the next paragraph we explain how to separate them. The total field distribution will be shown in the vicinity of a silicon/gold interface at the surface at and compared to the well-known Fresnel result one has in mind. With "Fresnel result" we refer to an "effective setup", where half of the sample consists of infinitely extended Si, the other half of infinitely extended Au, and the reflected fields are superimposed, *as if a linear combination would provide a correct description*. Secondly, the Jones reflection matrix for such a setup will be computed for various azimuthal angles to relate the effects to ellipsometric measurements. RCWA (and FEM) as a numerical technique delivers for each component i the position dependent total field components $E^{(i)}(x, y, z, t = 0)$ for all space points, either real or complex. The time dependence may then be incorporated into the result by multiplying with the harmonic oscillation.

The Jones matrix terms r_{ss}, r_{ps}, r_{sp} and r_{pp} are calculated numerically from the s- and p-scattered and incident field contributions over one period in the 0th order diffraction angle (i.e. specular reflection). As a side comment we mention that RCWA also allows to calculate the polarization response of any other diffracted order; this is naturally strongly wavelength dependent.

Because the reflected field, as well as the total electric field, becomes position dependent for an inhomogeneous sample – in addition to the phase factor $\vec{k} \cdot \vec{r}$ – the modified Fresnel coefficient r_{ab} ($a, b \in \{s, p\}$) where a and b are respectively the incident and reflected polarizations is also position dependent. Considering $r(x)$ as the ratio of the complex reflected field $E_r(x, y = 0, z = 0^+)$ to the incident field $E_i(x, y = 0, z = 0^+)$ at a given position of the surface, averaging over the unit cell, indicated by $\langle \cdot \rangle$, yields the measured

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