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Total Internal Reflection Ellipsometry of 2D Periodic Structures

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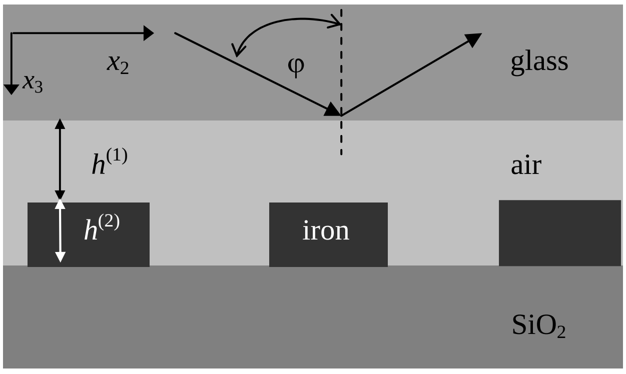
1. Introduction

There are many fields in optical research, sensorics or nano-technology, where the total internal reflection setup with coupling prism was found excellent applications [1–4]. Especially, the concept of total internal reflection ellipsometry (TIRE) can give answers to wide range of experimental and theoretical questions connected with nano-optical research – see [5] for instance and references therein.

In some of our recent works we have modeled various types of TIR systems with ellipsometric output. The influence of gap thickness and material properties has been analyzed for planar prism-gap-substrate system in [6] and [7]. An interaction of evanescent wave with periodic lamellar grating involving into the gap has been modeled in [8] and [9]. Here the effects have been studied that are connected with stripes geometry, and, with absorption in elements of grating.

In presented paper we analyze similar properties in the TIR structure containing two-dimensional periodic system of metallic square dots. Obtained results demonstrate the dependence of ellipsometric response on air gap thickness, and, also the comparison for planar, lamellar and 2D binary periodic system is reached. A short overview of our mathematical model based on the coupled-waves-method (CWM) is the objective of the next section; the main numerical results are summarized in the section 3 inclusive the discussion. The last part contains concluding remarks.

The basic parameters of considered TIRE system setup are analogous as in [8]. The high refractive index medium (coupling prism) is represented by the BK-7 glass. The binary grating created as Fe square dots on the SiO_2 substrate is separated from the prism by thin air gap. The geometrical characteristics of the periodical structure are showed in the Fig. 1: grating period Λ = 260 nm (the same in the directions x_1, x_2) and square dots size d = 130 nm do not change in the all samples. The thickness $h^{(1)}$ of air gap is the variable parameter whereas the dot height $h^{(2)}$ = 10 nm is fixed. All the materials are supposed to be isotropic. As the refractive index of prism, $n^{(0)}$, is larger than this one of air gap, $n^{(1)}$, the dependence of ellipsometric angles ψ, Δ on incidence angle φ upon the critical angle φ_c exhibits the specific feature that is typical for internal reflection.



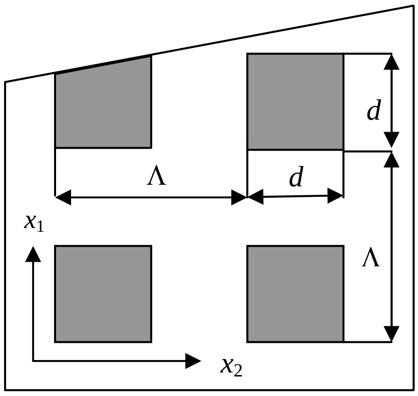


Figure 1: TIR multilayer scheme with geometrical and material characteristics.

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2. Theoretical model

Incident monochromatic plane wave with free-space wavelength λ propagates in homogeneous isotropic superstrate with refractive index $n^{(0)}$ under the angle φ in the plane $x_1 = 0$. The wave-vector in arbitrary νth layer is then written as

$$\mathbf{k}^{(\nu)} = k_0(\alpha_m, \beta_n, \gamma_{mn}^{(\nu)}), \quad \alpha_m = \lambda m/\Lambda, \quad \beta_n = n^{(0)}\sin\varphi + \lambda n/\Lambda, \tag{1}$$

where $k_0 = 2\pi/\lambda$ is the wave-number. The space-dependent part of electrical intensity (the time factor $\exp\{i\omega t\}$ is assumed) is represented by superposition of infinite set of partial polarization states of the form

$$\mathbf{E}^{(\nu)}(x_1, x_2, x_3) = \sum_m \sum_n u_{mn}^{(\nu)}\, \mathbf{e}_{mn}^{(\nu)} \exp\{-ik_0(\alpha_m x_1 + \beta_n x_2 + \gamma_{mn}^{(\nu)} x_3)\} \tag{2}$$

with unknown (except incident wave) amplitude coefficients $u_{mn}^{(\nu)}$, polarization vectors $\mathbf{e}_{mn}^{(\nu)}$ and propagation constants $\gamma_{mn}^{(\nu)}$. The last can be derived in any homogeneous region (superstrate, gap or substrate) by Rayleigh formula,

$$\left(\gamma_{mn}^{(\nu)}\right)^2 = (n^{(\nu)})^2 - \alpha_m^2 - \beta_n^2 . \tag{3}$$

However, in the periodically modulated layer the Fourier modal method (see [10], for instance) must be used that leads to certain eigenvalue problem producing eigen-polarizations and propagation constants. In the praxis, the calculation is realized over truncated mode set $-M \le m,n \le M$.

Boundary conditions on each interface and their one-to-other coupling generate system of algebraic equations for amplitude coefficients in the super- and substrate that reaches in discussed case the form

$$\mathbf{u}^{(0)} = \left(\mathbf{D}^{(0)}\right)^{-1} \mathbf{T}^{(1)}\mathbf{T}^{(2)}\, \mathbf{D}^{(3)}\mathbf{u}^{(3)} . \tag{4}$$

Any inner layer contributes in right-hand product by the matrix $\mathbf{T}^{(\nu)} = \mathbf{D}^{(\nu)}\left(\mathbf{P}^{\nu}\right)^{-1}\left(\mathbf{D}^{(\nu)}\right)^{-1}$, ν = 1, 2, where the matrices $\mathbf{D}^{(\nu)}$ are composed from polarization vectors, and, diagonal propagation matrices $\mathbf{P}^{(\nu)}$ have non-zero elements of the type $\exp\left\{\pm ik_0\gamma_{mn}^{(\nu)}h^{(\nu)}\right\}$. Note, that this approach is usually referred as the T-matrix algorithm [11]. The vectors $\mathbf{u}^{(0)}$ and $\mathbf{u}^{(3)}$ contain arranged coefficients of forward and backward waves for both principal polarizations *s*, *p*. Generally, it means the total dimension $4 \times (2M+1)^2$ for the problem (4).

Reflection properties of the TIR system at the zero mode order are defined for normalized input by complex ratio Ω that allows determining of ellipsometric angles ψ and Δ:

$$\Omega = \frac{u_{00,p}^{(0-)}}{u_{00,s}^{(0-)}}, \qquad \psi = \mathrm{arctg}\,|\Omega|, \quad \Delta = \arg\ \Omega . \tag{5}$$

3. Results and discussion

At given wavelength λ = 632.8 nm refractive index $n^{(0)}$ of the BK-7 glass was estimated by relation referred in [12], for the air gap $n^{(1)} = 1$. This one for iron was considered as $n^{(2)} = 2.87 - 3.46i$, refractive index $n^{(3)}$ of the SiO_2 substrate was computed using well-known Sellmeier's formula with the parameters $A = 1.1336$ and $B = 92.61$ [13]. Because of the small ratio $h^{(2)}/\lambda$ the truncation order $M = 5$ insured sufficient resulting precision for the 2D computation model, for which the step of incidence angle Δφ = 2° was established. Note, that the negative parts of Δ-curves are overturned into the region of 0° -180° in the following graphs.

Reflection response of a TIRE is significantly influenced by thickness of the gap between the coupling prism and tested sample. The penetration depth of evanescent wave for the wavelength 632.8 nm at incidence angle 70° is 49.7 nm in prism-air system, for instance. The sensitivity of total reflection ellipsometry in ψ and Δ for the binary grating with square metallic dots is demonstrated in the Fig. 2, where we can observe the combination of two effects. The first is the influence of the coupling strength, the second one follows from the material absorption of lossy dots.

The coupling strength between high index medium and 2D grating for 10 nm gap is characterized as strong [14]. As the consequence the shifts of ellipsometric angles from zero level and the expressive change in the ψ minima position for dielectric gratings have been described [8]. Since the critical angle for fictitious prism-substrate interface is 75.9 deg at mentioned wavelength, we can see significant increase of elipsometric values over this angle in the case of the smaller gap thicknesses. These theoretical results show the important condition for TIRE experimental arrangement – to realize the experiments with the air gap thickness not less than 30 nm. If the gap thickness is enlarged, the changes of elipsometric parameters become more expressive near the critical angle φ = 41.3° for the "pure" refraction from glass into the air.

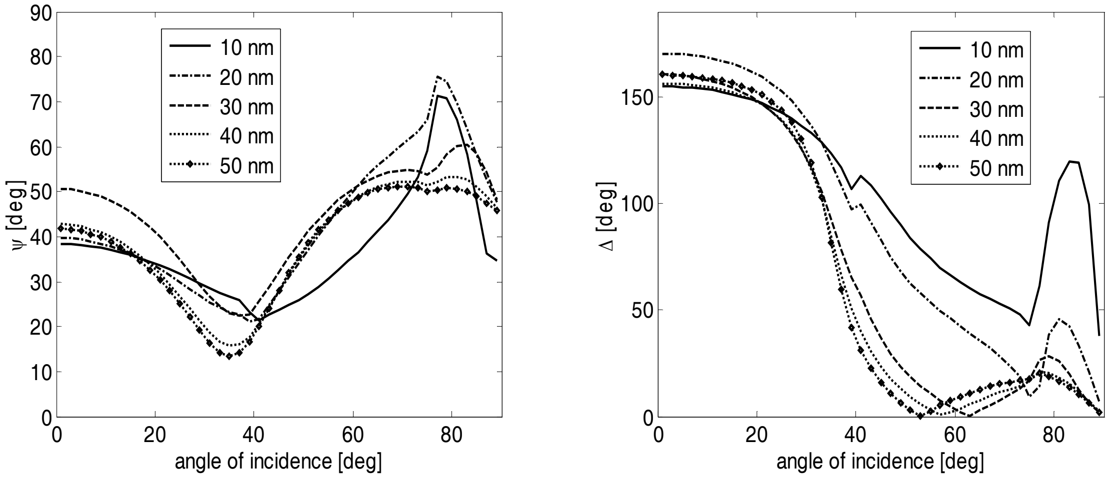

Figure 2: The dependence of ellipsometric angles on the air gap thickness.

The non-zero imaginary part of refractive index of metallic grating elements affects ψ and Δ parameters in the whole incidence angle range (see Fig. 2). However, this influence is again most apparent for the dots close to prism-air interface, and, beyond total internal reflection, where the expressive modification for ellipsometric angles can be observed. Very thin air gap (e. g. 10 nm) means the strong interaction of electromagnetic field with free electron medium.

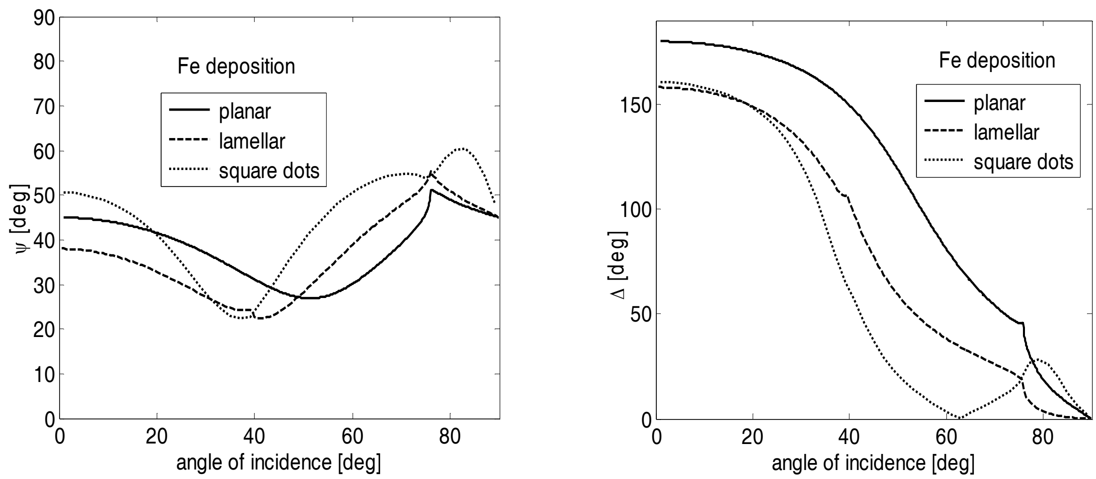

Figure 3: Comparison of TIRE systems with different structure of iron layer.

The comparison of spectral dependences of ψ and Δ ellipsometric angles of TIRE arrangement for thin metallic film system, and, for one- and two-dimensional gratings with metallic stripes and dots is demonstarted in the Fig. 3. The coupling strength has been fixed to the constant value related to the air gap thickness of 30 nm. The thicknesses of the metallic film, stripes and dots are the same – 10 nm. The theoretical results specify the influence of the fill factor in particular metallic structure. For our cases of the thin film, stripes and square dots these factors are 1, ½, and ¼, respectively. The Δ angles beyond the critical angle are importantly modified as function of fill factor (the left picture). For ψ dependences the minima shifts are again evident as in previous figure.

4. Conclusions

The modeling of total internal reflection ellipsometry demonstrates the extreme sensitivity of ellipsometric angles to the fill factor of the metallic grating elements, and, to the thickness of coupling gap. An interesting application is using this method for surface effects study especially for metallic and anisotropic media. The presented approach will be expanded in the near future to the 2D structures with anisotropic dots. This solution offers new possibilities in the area of space sensors and detectors, and, for solution of some scatterometric problems as well.

Acknowledgments

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