Light transmittance through a thin conducting film with various correlation between interface profiles

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Abstract. Light transmission through thin conducting films with determined and non-determined nanoscale profile relief has been considered theoretically. In the case of non-determined profiles our calculations are based on Green’s tensor techniques taking into account the first order perturbation theory, when the divergence of rough surface from flat is considered as perturbation. And in the case of determined and periodic profiles ones are based on differential formalism. There are two fundamental types of thin film profiles interaction, namely correlated and anti-correlated films. Both non-determined and determined periodic profiles of thin absorptive films demonstrate essential increase of obtained spectral and angular dependencies of the transmittance in the region of surface plasmon polariton excitation, especially for the case of anti-correlated film contrary to correlated one. It can be explained by complex coupling surface waves at different sides of film.

1. Introduction

Ebbesen et al [1] have discovered that the transmission of light through holes and their 2D periodic array with subwavelength diameters in a metal film can be strongly enhanced at the wavelengths of the surface plasmon polaritons (SPPs) excitation. These results have stimulated many subsequent experimental and theoretical studies of this phenomenon [2,3].

There are two regimes for excitation of SPP: 1) ordinary resonant SPP excitation appears under precision performance of the energy and momentum conservation laws and this case is characterized by non-monotonic peak-liked spectra, and 2) the non-resonant SPP excitation appears in system with the interface, space or material random inhomogeneities, and this regime is characterized by relatively monotonic optical spectra. These random inhomogeneities result in the essential broadening of SPP wave vector (for example, in the rough interface case the SPP broadening is determined by the inverse correlation length). There are correlated, anti-correlated and non-correlated principal types of stochastic correlation between both rough interfaces of absorptive film.

In this work we have presented the theoretical calculations of the transmittance of a thin absorptive film, deposited on a semi-infinite another absorptive (semiconductor) substrate with abovementioned correlation between film interfaces. Our calculations are based on the Maxwell’s equations solution in the framework of the Green’s tensor formalism in the first order of the perturbation theory, when the deviation of interface profiles from flat interface was considered as perturbation. Similar to roughness films we have investigated the influence of interfaces correlation on optical properties in the case of deterministic correlation too. And these calculations are based on the accurate solution of electrodynamics problem in curvilinear coordinates in the differential formalism like to C-method [4].

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2. Formalism

For simulation purpose we consider a corrugated thin absorptive film (metal) deposited on substrate (semiconductor) with the different interface profiles described by random or periodic profile functions $\xi_p(r)$ (see figure 1). We initialize Cartesian coordinate $z$ along the structure growth axis, so the numbers $z_p$ are denoted averaged positions of layers ($z_1=0$, $z_2=d$ for film with thickness $d$) and $p$ being interface and layer number. The thin film bounds are defined in the form: $z=z_p+\xi_p(r)$, where $r=\{x,y\}$ is in-plane coordinate vector (the space and inverse space coordinates are presented as $R=(r,z)$ and $K=(k,k^\perp)$ respectively). Also, we must assume that first layer is non-absorptive (dielectric or vacuum) and the film and substrate are homogeneous and isotropic, so layer permittivity, $\varepsilon_p$, are scalars.

![Figure 1. Scheme for absorbing (e.g. metallic) film on semiconductor substrate with two rough surfaces (with correlation (a) and anti-correlation (b) between interfaces).](image)

2.1. Integral formalism

We separate the permittivity of the considered structure (figure 1) on two terms: 1) the flat film permittivity in the form $\varepsilon(z)=\varepsilon_1(\theta(z))+\varepsilon_2(\theta(z))+\varepsilon_3(\theta(z-d))$, where $\theta(z)$ is the unit step function; 2) the deviation of the rough film permittivity from the flat one in the following form

$$\delta\varepsilon(r,z) = \sum_{p=1}^{2} (\varepsilon_p - \varepsilon_{p+1}) \left[ \theta(z-z_p-\xi_p(r)) - \theta(z-z_p) \right].$$

(1)

Considering the $\delta\varepsilon(r,z)$ as perturbation in the Maxwell’s equations system and using the Green’s tensor techniques [5], the electric and magnetic fields are expressed in the integral equation form

$$\begin{bmatrix} E(r,z) \\ H(r,z) \end{bmatrix} = \begin{bmatrix} E_0(r,z) \\ H_0(r,z) \end{bmatrix} + \sum_{p=1}^{2} (\varepsilon_p - \varepsilon_{p+1}) \int_{z_p}^{z} dz' \int_{z_p}^{z'} dz'' \begin{bmatrix} \tilde{G}_{EE}(r-r';z,z')E(r',z') \\ \tilde{G}_{HE}(r-r';z,z')H(r',z') \end{bmatrix},$$

(2)

here $E_0(r,z)$ and $H_0(r,z)$ are electric and magnetic fields for flat interface problem respectively, $\tilde{G}_{EE}(\Delta r;z,z')$ and $\tilde{G}_{HE}(\Delta r;z,z')$ are the Green’s tensors of the Maxwell’s equations for flat multilayer structure. In the perturbation theory framework we search solution in the first order form, where the integration over $z'$ can be performed analytically due to definition of Green’s tensors and fields $E_0$ and $H_0$ from flat interface problem.

For determination of transmittance/reflectance for considered system we use the Poynting’s vector, $S(R)>z=Re[E(R)\times H(R)]$ which one is averaged over the high-frequency period and the random profile ensembles (by $<...>$ is denoted the averaging over the random profile ensembles). The averaging of the Poynting’s vector over the random profile ensembles leads to statistical moments, which in the case of statistically homogeneous with statistically low irregularities grade (root-mean-square value is much less than the correlation lengths and wavelength) roughness with normal distribution of random value $\xi_p(r)$ can be expressed in the form

$$\langle \theta(\xi(r))\xi(r) \rangle \approx \frac{\sigma}{\sqrt{2\pi}} \cdot \langle \theta(\xi_1(r))\xi_1(r)\theta(\xi_2(r'))\xi_2(r') \rangle \approx \sigma_1 \cdot \frac{1}{\sqrt{2\pi}} \frac{W(r-r')}{4},$$

(4)

here $W(\Delta r)=\exp(-\Delta r^2/2l_0^2)$ ($W(k)=2\pi l_0^2 \exp(-k^2l_0^2/2)$ is one Fourier transformation) is the Gauss
correlation function, $l_\xi$ is the correlation length between random points on the same or different interfaces, $\sigma_\xi$ is the root-mean-square values of the rough interfaces. The sign “+” in (4) corresponds to the direct stochastic correlation between interfaces, $\xi_1(r) \approx \xi_1(r)$, and sign “-” corresponds to the inverse stochastic correlation (anti-correlation) between interfaces, $\xi_1(r) \approx -\xi_1(r)$, (see figure 1).

2.2. Differential formalism
We consider a corrugated thin absorptive film (metal) deposited on substrate (semiconductor) with the different interface profiles described by periodic functions with the same period (figure 1). Follow to C-method [4] we introduce two coordinate systems in which profile of each corrugated interfaces is transformed to flat profile. The sets of two types of curvilinear coordinates and their interrelations with Cartesian coordinates can be written in the form

$$
\begin{align*}
\bar{x}^1 &= x^1 = x; \quad \bar{x}^2 = x^2 = y; \quad \bar{x}^3 + \xi_2(x, y) = x^3 + \xi_1(x, y) = z.
\end{align*}
$$

The overlines denote the values, which correspond to lower interface of transition layer, and values without overline correspond to upper interface. The solution for Maxwell’s equations can be found in the form of the flat wave superposition with taken into account relief function periodicity.

3. Numerical estimations
The spectral dependencies of light transmission through a thin metal (Au) continuous film with 26 nm thickness onto GaAs substrate were presented in figure 2. The permittivities for Au and GaAs were taken from [6] and [7] respectively. These dependencies were calculated for the cases of the correlated, anti-correlated and non-correlated (random profiles at both film interfaces are independent $<\xi(r)\xi(r')>=0$) films at the different polarization of incident light. The increase of the transmittance in the negative real part of permittivity region (for Au at wavelength more than 500 nm) due to the interface anti-correlation can be explained as the SPP coupling at the energy conversion through thin film. This process can be presented in two stages, when incident light excites the film SPPs, which then decay into plane light waves. The increases of transmittance due to small roughness reaches about 10% as compared to that in the case of flat surface and essentially depend on rough interface correlation. This is in agreement with the experimental data for nearly smooth (nanorough) surfaces [8].

For examination of the influence of determined periodic interfaces on the light transmission we have chosen 1D profiled thin Au film on GaAs substrate with profile functions defined in the form

$$
\xi(r) = \pm \xi_\ell \cos(G_x r),
$$

where $2\ell$ is grating depth. The angular and spectral regions was chosen for observation SPP excitation peaks correspond to the $n=1$ diffraction order as follows from the momentum conservation law for SPP excitation, $k_{\text{SPP}} = k_x + n G_x$, where $k_{\text{SPP}}$ is SPP wave vector, $k_x$ is in-plane incident wave vector and $n$ is diffraction order. These dependencies demonstrate sufficient angular and spectral transmittance increasing, especially for anti-correlated relief.

**Figure 2.** Spectral dependencies for correction to s- (a) and p- (b) polarized light transmittance through Au film (26 nm) into GaAs substrate for 60° incidence in the cases of correlated (solid), anti-correlated (dash) and non-correlated (dot) random interface profile (roughness parameters: $\sigma=5$ nm $l_\xi=100$ nm).
λ = 632.8 nm

**Figure 3.** Angular (for 632.8 nm incident wave) and spectral (for 13° incidence angle) dependencies for full transmittance trough Au film with 50 nm thickness to GaAs substrate for the cases: correlated (dot), anti- correlated (dash) and flat (solid) film interfaces with the 25 nm relief depth.

### 4. Discussions and conclusions

Within the framework of the classical electromagnetic theory (when the light interaction with medium is considered phenomenologically), the increase of the light energy transmitting through thin metallic films due to anti-correlation between thin film interfaces was obtained theoretically. The Green’s tensor technique in the perturbation theory framework was used in the stochastic correlation case, while the differential formalism like to C-method [4] was used in the deterministic correlation case. Overall calculations demonstrate transmittance increase at the inclined incidence especially for \( p \)-polarized wave in the anti-correlated films case, which can be explained by excitation of the coupled film SPPs of two opposite surfaces.

By analogy to the works [9,10], the transmittance increase could be explained in the following steps of interaction: 1) the conversion of volume electromagnetic waves taking place in air into the surface wave at the "air-absorptive film" rough interface; 2) coupling the surface waves at the "air-absorptive film" and the "absorptive film-substrate" interfaces due to the stochastic correlation between ones; 3) the conversion of surface waves at "absorptive film-substrate" rough interfaces to volume waves in the substrate.

This theory may be of use when analyzing the photocurrent spectra in solar cells of the Schottky-diode type when a thin semitransparent high conducting film of indium-tin-oxide (ITO) or metal is used as some frontal electrode. It allows to more correctly determining their internal quantum efficiency and recombination parameters of interfaces [11].

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