Mathematical modelling of thin films growth and calculation of coefficients reflection, transmission and absorption waves

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Mathematical modelling of thin films growth and calculation of coefficients reflection, transmission and absorption waves

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Abstract. Progress in nano- and microsystem technology is directly related to the development of thin-film technologies. At the present time, thin metal films can serve as the basis for the creation of new instruments for nanoelectronics. One of the important parameters of thin films affecting the characteristics of devices is their optical properties. That is why the island structures, whose optical properties, can change in a wide range depending on their morphology, are of increasing interest. However, despite the large amount of research conducted by scientists from different countries, many questions about the optimal production and use of thin films remain unresolved.

1. Introduction
The quality of many famous materials can be enhanced by using nanoparticles and atomic processing. Nanotechnology make it possible to create lighter, thinner and stronger composite (mixed, compound) materials.

To study nanostructures, it’s important to know not only their mass or arrangement of atoms, but what they consist of. Determine the chemical composition of the samples (i.e. the content atoms of various elements in them) are allowed spectroscopic methods that use various instruments for studying the spectra of radiation, absorption, reflection, scattering.

As is known, ordinary light (visible radiation) is a collection of electromagnetic waves of different lengths (~ 400-760 nm) perceived by the human eye. Our eye perceives different colors not because objects have some abstract property "color", but because they are able to absorb and reflect electromagnetic waves of some length.

The analysis of the spectra of optical transmission and reflection plays a primary role among various methods of investigating quantum-size structures.

The characteristics of a number of optical elements, which include interference coatings, including a metal layer, are significantly influenced by the parameters of thin metal layers (refractive index, main absorption index and thickness). To this group of optical elements are mirrors, both metal and metal-dielectric, attenuating optical filters for a wide spectral range, gradient attenuators (shaders) and metal-dielectric narrow-band filters. The characteristics of each of the listed elements (transmission, reflection) are to some extent influenced by the optical parameters of the metal layers, which in turn depend on the deposited material and the resulting morphology of the sample surface.

The morphology of the surface of thin films is one of the most important parameters. That is why there is an increasing interest in the structure of islands, their roughness and thickness. Today, obtaining thin films is unthinkable without the use of mathematical modeling, numerical methods and complex
programs. In this study, the degree of influence of morphology (particle diameter, number of layers, etc.) on the optical properties of a deposited thin film of bimetallic clusters was studied.

2. Computer modeling

For computer modeling of the growth of metal thin film, a mathematical model of the "cellular automaton" type was used, which has recently been widely used in modeling processes in nanotechnologies.

The growth model of a granular film in the form of a deterministic cellular automaton consists in depositing particles on a substrate randomly. Each particle hits random points on the substrate and is fixed there, increasing at a given point the thickness of the resulting film by one relative unit.

For research the optical properties of modeled structures, the Finite Difference Time Domain method (FDTD) was used, which is one of the most popular methods of numerical solution of Maxwell's equations. Since introduction in 70th years of the previous century this method became popular due to it certain advantages:

- Simplicity of explicit numerical scheme;
- High parallel efficiency;
- Easiness of complex geometry generation;
- Ability to handle dispersive and nonlinear media;
- Natural description of impulsive regimes.

FDTD includes various numerical techniques and options, such as algorithm for dispersive and nonlinear media modeling, different mesh types, simulation results postprocessing etc.

We list the "main participants" of the FDTD numerical experiment:

- Material bodies, whose optical properties we are investigating.
- The source of the electromagnetic wave. The simplest way to specify a source is to specify the time dependence of in Maxwell's equations. This type of source is usually used in simulating dipoles. To generate a plane wave, another type of source that is implemented using the total field / scattered field method is more convenient.
- Detectors that remove fields on the grid during the entire numerical experiment. Detectors are not responded to by any real bodies in space, by which is meant only that we write the values of the fields at some points inside the computational volume into a file. Upon completion of the calculation based on this file, you can restore the course of the numerical experiment.

The medium (material) of objects is described by dielectric permittivity, conductivity, magnetic permeability and magnetic losses. Their default values are \((1, 0, 1, 0)\). Unlike frequency domain methods, the dielectric permittivity of dispersive materials in tabular form can't be directly replaced by the FDTD scheme. Instead, it can be approximated with the help of several members of Drude or Lorentz in the form:

\[
\varepsilon(\omega) = \varepsilon_\infty - \sum_{p=1}^{N_D} \frac{\Delta \varepsilon_p \omega_p^2}{i\omega \gamma_p \omega_p} + \sum_{p=1}^{N_L} \frac{\Delta \varepsilon_p \omega_p^2}{\omega_p^2 - 2i\omega \gamma_p - \omega^2}
\]  

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\]  

The Total Field/Scattered Field method is used to simulate an infinitely distant plane wave source. It's based on the linearity of Maxwell's equations and the following superposition principle. FDTD difference equations can be independently applied both for the total field and for the incident or scattered fields, which allows us to break the computational volume into the field of the total field and the region of the scattered field. They are separated by a virtual boundary, which serves to generate a plane wave in the region of the total field. The difference equations used to calculate the field components in the grid nodes adjacent to this boundary differ from the original ones by the presence of additional components that take into account the value of the field of the incident wave.
To simulate the departure of a wave from the computational volume to infinity, absorbing boundary conditions are required. One of the best implementations is the use of a thin layer of special material called the Perfectly Matched Layer (PML) along the boundary. Thus, this material absorbs all waves incident on the boundary of the computational volume, regardless of the angle of incidence. To model infinite periodic structures, periodic boundary conditions are used in one or several directions.

In order to measure the fields inside the computational volume, detectors are needed. They read the values of the fields at the points where they are placed, without affecting them at all. The values on the detectors are obtained by interpolation at nearby grid nodes. In the course of a numerical experiment, detectors record their readings in binary files. At the end of calculations, based on these binary files, readable text files are created.

In EMTL there are different types of detectors which can be divided into two groups: universal and special detectors. At the same time, it is customary in EMTL to operate not with separate detectors, but with sets of detectors.

A universal detector records the history of the signal in the form of a table with columns \( t, x, y, z, E_x, E_y, E_z, H_x, H_y, H_z \) for time, coordinates and values of fields \( E \) and \( H \).

A special detector creates input files with time, coordinates and \( E \) and \( H \) field values for plotting and 3d views. Special detectors include: NearToFar - used to convert fields from near field to distant; RTA - is used to measure the passage, reflection and absorption of a signal from a structure; Flux - used to measure energy flows through surfaces.

Typical scenario of FDTD experiment includes following steps:

- User specifies calculated volume and mesh resolution, optical properties and geometry of the structure, boundary conditions (typically, periodic or absorbing), wave source and set of points where field values should be recorded (detectors).
- Source generates finite time width impulse impinging on structure. Its propagation and scattering is recorded by detectors and possibly transformed to the frequency domain. Total exit of the radiation through absorbing boundaries determines the simulation time.
- Recorded field values are processed (for example, energy flux integrating through the chosen surface) to get optical characteristics of the structure.

### 3. Results of modelling

Using the FDTD method: a plane wave propagates along the Z-axis and automatically calculates the energy flux for the transmitted (\( T \)) waves using the data from the detectors.

![Figure 1. Transmission spectra of the deposited films: 1 – Au:Ag(1:1), a particle diameter (D) is 50nm, one layer, the distance between particles (gap) - is 5nm; 2 – Au:Ag(1:1), D is 10nm and five layers, gap is 4nm; 3 – Au:Ag(1:1), D is 10nm and five layers, gap is 2nm.](image-url)
Using the data from the detectors, it’s also possible to calculate the coefficients of the reflected (R) waves. Absorption (A) is obtained as $A = 1 - R - T$.

Figure 1 shows the transmission spectra of deposited bimetallic films and transmission spectra obtained with the help of FDTD of simulated thin films.

The calculated transmission spectra are in qualitative agreement with the experimental data.

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