Numerical calculation of asymmetric antireflection microstructures spectral transmission dependency on polarization

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Abstract. In this paper we performed a numerical analysis of middle infrared antireflection microstructures with elliptical holes. We used COMSOL Multiphysics finite element method analysis commercial software. The calculation results revealed the qualitative influence of structure surface imperfections and non-symmetry on transmission spectra for different polarizations. This fact has to be taken into account for the design of polarization-independent antireflection microstructures.

1. Introduction

Materials like germanium, silicon, sapphire, zinc selenide, zinc sulfide, cadmium sulfide and cadmium selenide are widely used for making modern middle infrared (mid-IR) optical instruments. Refractive index of these media varies from 2 to 5 in mid-IR range. Due to that, there are surface reflection losses up to 30\% per surface. These losses can be reduced or even eliminated in relatively wide range of wavelengths and angles of incidence by using thin film antireflection coatings [1]. Nevertheless, coatings have such disadvantages as vulnerability to surface contamination and thermomechanical damage. These coatings also have lower light-induced damage thresholds than the substrates on which they are deposited [2].

There is an alternative to traditional thin film coatings. The idea is to make the transition between two media steep enough to eliminate reflection [3]. For that purpose, one can use antireflection microstructures (ARMs) [4]. ARMs are surfaces that have been patterned using periodic structures with different cross-section profiles. The typical height of these structures is a few microns and their period is dependent on the wavelength range in which increased transmission is required. The microstructure antireflection principle can be described using effective medium theory [5] for wavelengths longer than

\[ \lambda = np \]  

where \( n \) is the refractive index of the material and \( p \) is the microstructure period. However, implemented methods of ARMs fabrication have various disadvantages. The main disadvantage is the complexity of the technological process. It is important because ARM optical properties can differ depending on the fabrication process. In the BMSTU we developed a new method of microstructure fabrication [6]. This method is relatively simple, but the first examinations of transmission spectra showed its polarization dependency. That can only occur due to the imperfection of ARM geometry like eccentricity of holes shape. We performed numerical calculations to estimate the polarization dependency on the ARM surface morphology.
2. Numerical calculation setup

For the numerical calculation we used finite element (FEM) software COMSOL Multiphysics. The model setup is typical for electromagnetic calculations of spatially periodic subwavelength structures. The calculation volume contains one period of microstructure with with Floquet periodic boundary conditions (FPBC) applied to its sides and with perfectly matched layers (PML) from top and bottom (see figure 1).

Source and receiver ports were placed at some distance from PMLs to avoid artifacts in transmission calculation. The geometry of structure was derived from averaged atomic force microscope (AFM) images (one of them is shown in figure 2) of structure fabricated on CdSSe crystal surface. Thus, material refractive index was set to 2.35 to match the refractive index of CdSSe mid-IR range. The medium was air with refractive index of 1. Average ARM depth was 1.35 µm and the period was about 1.7 µm as measured using AFM. Holes of structure are elliptical with average measured minor to major axis ratio of 0.84. AFM scanning height resolution is 10 nm but after averaging and smoothing the mesh it degraded down to near 50 nm.

The FEM calculation was performed in range from 3 to 14 µm with 0.1 µm step which is sufficient to simulate general behavior of transmission spectrum in mid-IR. The mesh element size was 1/25 of shortest propagating wavelength (0.12 µm). The chosen size provides reasonable accuracy for transmission calculation even for a complex large-scale AFM-imported geometry. That fact was verified on simpler models with already known output to match it with less than 1% relative error. Moreover, mesh size exactly near the surface of structure were scaled by a factor 0.4 to match the resolution of AFM scans and correctly take into account possible near-field interactions.
3. Results and discussion
Calculated transmission for two electromagnetic waves of orthogonal polarizations is shown in figure 3. X-polarization oriented along minor axis of structure elliptical holes while Y-polarization oriented along major axis.

![Figure 3](image.png)

It can be clearly observed that transmission is highly dependent on polarization. The difference between two transmission spectra reaches 5% and their transmission maximum peaks is shifted from each other by 1.9 µm. We believe that this is due to the difference in effective refractive index gradients for two polarizations. Figure 3 also shows that the average of two polarizations closely matches the measured transmittance for non-polarized light.

4. Conclusion
The numerical calculation performed in this paper illustrates how transmission spectra of antireflection microstructures depend on their elementary cell geometrical symmetry and in this particular case – on holes’ eccentricity. These results can be useful for designing both antireflection and polarization microstructures for the use in the mid-IR range.

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