Spectral Fourier-microscopy of the periodic structures based on Ge$_2$Sb$_2$Te$_5$

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Abstract. The method of spectral Fourier microscopy was used to study the reflection spectra with an angular resolution of submicron periodic gratings based on amorphous and crystalline Ge$_2$Sb$_2$Te$_5$. The form of the dispersion curves of quasi-waveguide modes in the structures under study was established. The experimental data were compared with the calculations of dispersion curves in synthesized diffraction gratings. Reasonable agreement between theoretical and experimental data was obtained.

1. Introduction.
Phase-change memory materials based on complex chalcogenides of the Ge-Sb-Te system are promising media for tailoring metasurfaces of various configurations [1–4]. Such structures can serve as a platform for the creation of new control elements for light flows by changing the phase state of the material under various external influences [5–10]. In this work, we fabricate metasurfaces which are systems of submicron gratings based on amorphous and crystalline Ge$_2$Sb$_2$Te$_5$ (GST). It is shown, that quasi-waveguide modes can be efficiently excited in such structures, which in turn leads to the appearance of narrow resonances (Rayleigh and Wood anomalies) in the optical response of structures at certain frequencies and wave vectors. The angular dependences of the observed peaks in the reflection spectra are investigated by the method of spectral Fourier-microscopy. The experimental data are compared with the calculated dispersion curves in the studied metasurfaces.

2. Samples.
Amorphous GST thin films were deposited onto the fused quartz substrate by magnetron sputtering of the stoichiometric polycrystalline target. The atomic force microscopy technique was employed to investigate the thickness (250 nm) of deposited thin film. Elemental
composition of the films was evaluated using the Auger spectroscopy (Physical Electronics PHI-660). The results showed that the composition of the deposited thin films was close to that of Ge$_2$Sb$_2$Te$_5$ and had a uniform distribution across the film thickness. The crystalline phase of GST thin films was prepared by annealing at 250 °C in argon.

For the grating fabrication, one step of 50 kV Crestec CABL-9050C e-beam lithography was used. Spin-coating of electronic resist ma-N 2403, e-beam writing of the gratings and their development in a ma-D 525 solution for 30 seconds with water as a stopper were performed. The reactive ion etching of GST film inside Corial 200 setup in SF$_6$ gas atmosphere was in situ monitored by a built-in reflectometer. Additionally, the etched devices were inspected by the broadband Filmetrix F-20 UVX reflectometer in grating-free places. By removing the rests of electronic resist in N-Methyl-2-pyrrolidon (NMP) the device fabrication was finalized. As a result, the structures with the period $P = 700$ nm and the stripe widths $w = 500$ nm were tailored. Examples of the fabricated gratings are depicted in Fig. 1 for amorphous (a) and crystalline (b) samples, correspondingly.

### 3. Methods

We used the method of spectral Fourier-microscopy to measure the angular dependencies of the reflectance. The method is based on the property of the lens to produce a Fourier transform of the light beam and makes it possible to measure the spectral-angular dependencies of the reflection coefficient without any displacement and rotation of the sample under study and the
source [1]. The focal lengths and the distances between the lenses in the optical scheme of the setup were selected in such a way that the Fourier image of the object under study was projected onto the surface of the CCD matrix. The measuring part of the setup consisted of an Acton SP2500 monochromator with a grating of 300 g/mm, and equipped with a Pixis 256E silicon CCD. The spectral range of measurements was 400-1000 nm, the angular range was ±50 degrees and was determined by the numerical aperture of the micro-objective used.

Theoretical calculations of the spectra were carried out by the Rigorous coupled-wave analysis method (RCWA) in the form of scattering matrices [11]. In numerical simulations we used a model of the structure depicted in Fig. 1(c). The method is based on dividing the structure into elementary planar layers homogeneous in the Z direction and two-dimensional periodic in the X and Y directions. The solution of Maxwell’s equations for each layer can be found in the form of Fourier-Floquet modes (plane waves). The exact solution can be thought of as an endless series of such modes [12]. The complex dielectric permittivities of the amorphous/crystalline GST films were determined from measurements by the spectral ellipsometry technique using a five-layer model (air - surface - GST - SiO$_2$ - Si) and a single Tauc-Lorentz oscillator (Fig. 1(d)).

4. Results and discussion

The experimental and theoretical reflectance spectra of the structures under study collected at different angles of incidence in p-polarization are presented in Figures 2,3 as two-dimensional functions of wavelength and incident angle for amorphous and crystalline states, correspondingly. There are minima and maxima forming tracks whose spectral position shifts to the long-wave region as the angle of incidence increases. It is noted that the theoretical and experimental spectra are in reasonable agreement with each other.

The observed tracks can be attributed to Rayleigh (rings) and Wood (stars) anomalies. Rayleigh anomalies describe by equation [13]:

$$n_{diffr} \sin \theta_{diffr} = n_{inc} \sin \theta_{inc} \pm m \lambda_r / P,$$

where $m$ is an integer referring to the order of the diffracted wave, $n_{diffr}$ and $\theta_{diffr}$ are the refractive index and diffraction angle in the substrate (SiO$_2$), $n_{inc}$ and $\theta_{inc}$ are the refractive index and incident angle in the external medium (air) and $P$ is the period of the structure. Rayleigh anomaly, appearing when $\theta_{diffr} = 90^\circ$, causes a dip in the transmission spectrum of light because the diffracted light propagates parallel to the grating. The observed Rayleigh anomaly is purely geometric and does not depend on the material of the diffraction grating. The angular and spectral positions of the anomaly will be determined by the grating period and refractive index associated with light diffraction into the air (blue rings, $n_{diffr} = 1$) and into the substrate (red rings, $n_{diffr} = 1.5$). For the structure under study at normal incidence of light, the Rayleigh anomaly associated with the first order of diffraction into air will be observed at a wavelength of $\lambda_r = 700$ nm. Thereby, it provides an efficient way to determine the exact angular position of the measured spectrum. For diffraction into the substrate, the spectral position of the Rayleigh anomaly is at the wavelength $\lambda_r = 1024$ nm, which is beyond the sensitivity limits of our experimental setup.

The Wood anomalies originate from the quasiguided modes which appear in the GST grating. Spectral position of the Wood anomalies can be approximated by equation [14]:

$$\lambda_w = \frac{2\pi}{G} \sqrt{\frac{\sin^2 \theta + (n_{eff}^2 - \sin^2 \theta)(1 + a)}{1 + a} - \sin \theta}.$$

Here, $\lambda_w$ is spectral position of Wood anomaly peak, $G = 2\pi / P$ is vector of the reciprocal lattice with period $P$, $\theta$ is angle of incident light, $n_{eff}$ is effective refractive index of the waveguide layer, and $a = (k_z / G)^2$. 
In this approximation, we consider the new effective structure consisting of homogeneous isotropic layers (silica/GST/air) corresponding to the consecutive steps of the staircase representation of the structure (Fig. 1(c)). The effective dielectric permittivity of the structure can be calculated by the effective medium theory \[ \varepsilon_{\text{eff}} = \frac{\sum \gamma \varepsilon_\gamma f_\gamma}{\sum \gamma f_\gamma}, \] where \( \varepsilon_\gamma \) is the refractive index of \( \gamma \)-th component in a layer, and \( f_\gamma \) is the filling factor of the \( \gamma \)-th component.

Diffraction anomalies studied in this work have a Fano line profile (Figures 2, 3) since they originate from the interference of the discrete quasiguided modes with a nonresonant light scattered by the structure. The difference in intensities (see Figs 2(a) and 3(a)) observed in the experimental spectra (peaks/dips at the same wavelengths and angles) may be due to a change in the Fano coupling parameter \[ \text{[16]} \] for amorphous and crystalline samples under investigation.

It should be also noted that there is only a slight change in the spectral position of Wood’s anomalies due to the GST phase state. We associate this observation with a small difference in the values of dielectric permittivities in the visible diapason of the wavelengths (see Fig. 1(d)). In the future, we plan to expand the spectral range of measurements to the practically important IR region of 1.5 \( \mu \)m (Telecom Standard), where the absorption is low and the refractive index changes from 4 to 7 under the GST phase transition from the amorphous to the crystalline state.

**Figure 2.** Experimental (a) and theoretical (b) angle-resolved reflection spectra for amorphous phase. The term ”Rayleigh air-to-air anomaly” refers to the diffraction of a plane wave into the environment (air). Accordingly, the term ”Rayleigh anomaly air-SiO\(_2\)” means the diffraction of a plane wave from air into a substrate (silica).

**Figure 3.** Experimental (a) and theoretical (b) angle-resolved reflection spectra for crystalline phase.
5. Conclusion
Metasurfaces in the form of diffraction gratings of amorphous and crystalline Ge$_2$Sb$_2$Te$_5$ with a submicron period (700 nm) were tailored by magnetron sputtering with subsequent electron lithography. Angle-resolved reflectance spectra in p-polarization were measured by Fourier imaging setup.

The experimentally observed resonance features in the spectra are interpreted as Rayleigh and Wood anomalies, the appearance of which is due to the excitation and propagation of quasi-waveguide modes in the near-surface region of the structures. The measured reflection spectra of the GST metasurfaces are in quantitative agreement with the simulation results obtained by the scattering matrix method.

The unique properties of the GST-based phase-change metasurfaces clear the way for the potential practical applications of such structures for all-optical switches in IR range corresponding to Telecom standard region (1.5 µm).

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