Reflection spectra of a thin-film GeSbTe diffraction grating on a silicon nitride waveguide

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Abstract. Recent advances in nanophotonics are due to the implication of new approaches to the photonic devices and components design, not only related to structural features, such as subwavelength periodic arrangements, but also new materials, e.g., phase-change materials like GeSbTe (GST) alloys. We consider recently proposed optical non-volatile GST memory cell with a GST diffraction grating instead of a continuous film placed on a silicon nitride waveguide. The grating allows diminishing the energy budget of an incident electromagnetic beam in case of an optically induced phase transition of GST due to excitation of the resonant guided mode in the grating. The excitation of this mode results in anomalous reflectance spectra of the waveguide-grating structure. Here, we present the reflection spectra of GST diffraction gratings on a silicon nitride waveguide calculated with the use of the matrix Riccati equation technique in the theory of multiple electromagnetic wave scattering in inhomogeneous media. We show how the reflection changes with variation of different parameters – grating period and height, incident wave polarization, and phase of the GST film.

1. Introduction
Nanophotonics is a rapidly growing interdisciplinary research field [1] that emerged as an alternative to modern nanoelectronics, which faces certain problems in progressing through the scaling of standard planar CMOS technology [2]. Nanophotonics provides exceptional opportunities for developing high-performance devices for optical telecommunications, computing, quantum cryptography, as well as for biological and medical applications [3]. In particular, it is anticipated that the integrated photonics and phase-change materials (PCMs) [4, 5] enable the development of a photonic non-volatile memory [6], which is essential to overcome the so-called von-Neumann bottleneck meaning the information traffic jam between the processor and the memory.

To store data, PCM-based electronic random access memory (PRAM or PCRAM [4, 6]) exploit the large contrast in electrical resistance between the amorphous state and the crystalline state of PCMs [4]. Typical PCM materials, such as chalcogenide glass compounds (GeSbTe, AgInSbTe etc.), are characterized by fast and reversible phase transitions between the two above-mentioned states at elevated temperatures. Thus, PRAM utilizes only the electrical properties of PCMs, and being an electronic component, it possesses the same disadvantages as all electronic devices compared to photonic ones, namely significant RC-delays, Joule heating, and low resistance to external electromagnetic (EM) radiation.
PCMs also demonstrate a large difference in refractive index upon a phase transition, an effect that has led to their commercial use in optical storage disks [7]. The concept of memory operation in optical disks relies on the far-field optics, which makes downscaling of such memory cells a challenging issue that requires the overcoming of the diffraction limit. On the other hand, photonic PCM-based non-volatile memory is operated in the optical near field, meaning that the sizes of memory cells are not restricted by the diffraction limit and can be reduced to nanoscales. Therefore, it allows avoiding the above-mentioned drawbacks of electronic devices.

Figure 1 illustrates the concept of a photonic memory cell proposed in [6]. A nanoscale GST film is placed directly on top of the waveguide. The guided mode is evanescently coupled into the GST film. Depending on the phase of the GST, the mode energy is absorbed inside the film to less (in the amorphous state) or greater (in the crystalline state) extent. Accordingly, the signal at the waveguide output weakens slightly in the first case and significantly in the second, thus, defining the levels of logical ‘1’ and ‘0’. The state of a GST film can be changed with the use of a more intense light pulse needed to heat the GST to the transition temperatures, providing ‘Write’ and ‘Erase’ operations. It is further reported that even intermediate crystallization/amorphization states of a GST film can be achieved, allowing for a multilevel cell that can be used as a memristor for neural network and artificial intelligence applications.

In this report, we propose a GST film in the form of a strip-like diffraction grating (figure 2) and numerically investigate the reflection of an EM wave from a waveguide-grating structure.

Using a grating instead of a continuous film has a three-fold aim. First, it allows diminishing the energy budget of an incident EM beam in the case of an optically induced phase transition of GST. Second, the evanescent part of the guided mode could be more strongly coupled to the grating. Third, the phase state of PCM may be simply verified on the basis of magnitudes of angular orders in the reflection spectra of relatively weak external EM radiation.

Indeed, it is well known that under certain conditions, a resonance phenomenon occurs in waveguide-grating structures comprised of a substrate or a thick buried oxide layer (SiO$_2$ in figure 2),
a thin waveguide layer (Si$_3$N$_4$), and a layer in which a grating is fabricated (GST). Hessel and Oliner demonstrated the resonant excitation of surface waves in metallic grating structures [8]. Neviere generalized this picture to deal with structures that include gratings and dielectric waveguides [9]. Later on, it was confirmed both numerically [10, 11] and experimentally [12] that the excitation of a guided mode in the waveguide and even in the grating layer itself [13] exhibits anomalous (maxima) zeroth-order reflections in the reflection spectra of the waveguide-grating structures. The latter case [13] is the most interesting in terms of the PCMs phase state because the above-mentioned resonant excitation of waves in the grating causes an increase in the incident EM wave energy absorption in the PCM grating strips.

2. Matrix Riccati equation method

We calculate the reflection spectra and the EM field spatial distributions for the waveguide-grating structure shown in figure 2 applying an analytical approach of “transfer relations” and “invariant embedding” method to the theory of EM wave multiple scattering in inhomogeneous media [14, 15]. This method uses the Riccati type equation for the matrix wave reflection coefficient and the associated differential equation for the matrix wave transmission coefficient. It allows considering the effects of strong energy transformations between homogeneous and evanescent waves in the near wave zone of the grating, which appear due to the subwavelength or comparable to the wavelength dimensions of the considered structures.

Let us assume that a plane TE polarized EM wave with wavelength $\lambda$ is incident from a background dielectric medium, $\varepsilon_{bg} = 1$, on a periodic structure with period $\Lambda$, height $h$ and dielectric permittivity $\varepsilon(\mathbf{r}, \omega)$ as a function of coordinates $\mathbf{r}$ and incident wave frequency $\omega$, at an angle of incidence $\varphi$ (see figure 2). The method of transfer relations allows representing the electric field of reflected and transmitted radiation as a superposition of the plane waves with certain wave vectors ($k^\mu_\nu$) and certain coefficients ($R_{\mu \nu}$, $T_{\mu \nu}$):

$$E_z(r) = \begin{cases} \exp\left(ik_0(r - hn_z)\right) + \sum_{\mu = -\infty}^{\infty} R_{\mu 0}(h)\exp\left(ik^+_\mu(r - hn_z)\right), & z > h \\ \sum_{\mu = -\infty}^{\infty} T_{\mu 0}(h)\exp\left(ik^-_\mu r\right), & z < 0 \end{cases} \quad (1)$$

$$k^\pm_\mu = \begin{pmatrix} \beta_\mu & 0 \\ 0 & \mp\sigma^\mu_\nu \end{pmatrix} = \begin{pmatrix} k_0\sin\varphi + 2\pi\mu/\Lambda \\ 0 \\ \pm\sqrt{k_0^2 - \beta^2_\mu} \end{pmatrix} \quad (2)$$

The reflection and transmission coefficients are derived from the solution of the following matrix differential equations:

$$R'_\mu = RA(z)R + \left(A(z) + C\right)R + R\left(A(z) + C\right) + A(z), \quad (3)$$

$$T'_\mu = T\left(A(z) + C + A(z)R(z)\right), \quad (4)$$

$$R, T\big|_{\mu = 0} = R_0, T_0, \quad (5)$$

where $R$, $T$, $A$, and $C$ are $(2n + 1)\times(2n + 1)$ -dimensional matrices with complex values and $n$ is selected in a special way to achieve convergence. The components of the matrices $A$ and $C$ are defined as follows:

$$A_{\mu \nu}(z) = i\frac{2\pi}{\lambda^2\sigma^\mu_\nu} f_{\mu \nu}(z), \quad (6)$$

$$C_{\mu \nu} = i\sigma^\mu_\nu \delta_{\mu \nu}, \quad (7)$$

and $f_{\mu}(z) = \frac{\pi}{\Lambda}\int_0^\Lambda \delta(x, z)\exp\left(-i\frac{2\pi x}{\lambda}\right)dx$ is a transformation function, it describes the interaction between propagating and evanescent waves at multiple scattering in periodical inhomogeneous media.
For TM polarization equations (3)–(6) and transformation function slightly differ. A more detailed description of the method is provided in [15].

3. Results and discussion

The reflection spectra (figure 3) of the GST diffraction grating on a 220 nm thick Si$_3$N$_4$ layer and SiO$_2$ substrate and spatial EM field distributions (figure 4) are computed for 1550 nm wavelength at normal incidence ($\varphi = 0$) and different parameters (the grating height and the period, the phase state of the GST material, TE and TM polarizations of the incident light). The grating period is varied from 0.2$\lambda$ to 10$\lambda$ (from 0.31 to 15.5 $\mu$m), height – from 5 to 70 nm, grating cycle ($a/\Lambda$) is maintained 0.5. The refractive indices of SiO$_2$ and Si$_3$N$_4$ at a given wavelength are 1.466 and 1.996, respectively. The refractive indices and the absorption coefficients of GST in the amorphous and crystalline states are $n_a = 4.4$, $k_a = 0.2$ and $n_c = 7.2$, $k_c = 1.4$, respectively, at the same wavelength [16].

![Figure 3(a, b, c, d).](image)

Figure 3(a, b, c, d). Reflection spectra of a thin-film GST diffraction grating on Si$_3$N$_4$ waveguide on SiO$_2$ substrate in the case of TE (a, b) and TM (c, d) polarizations of a normally incident plane wave for the amorphous (left side – panels a, c) and crystalline (right side – panels b, d) phases of GST at different grating heights ($h$ in nm). The dashed horizontal line indicates a “zeroth” reflection level of the Si$_3$N$_4$ layer on SiO$_2$ substrate without a grating.

Each graph in figure 3 shows a common sharp decline at a point $\lambda/\Lambda = 1.466$, which defines the (lower) boundary of the “subwavelength” regime of a grating [17]. Interestingly, this sharp decline is
typically followed by a more or less sharp increase in the reflectance (see figure 3a, 3c and 3d). However, the grating in the crystalline phase in the case of TE polarization (figure 3b) demonstrates a substantially different behavior resulting in at least three types of curves: first, lines with steep growth and a corresponding decrease (heights from 5 to 15 nm); second, lines with steep growth and a gradual decrease (heights from 20 to 30 nm); and third, lines with a sharp increase and an extra inflection followed by even a more gentle decrease (heights 40, 50 and 70 nm).

Another notable point is $\lambda/\Lambda = 1.0$ that defines the first Wood–Rayleigh grating resonance [18], also known as a “mode opening” and physically meaning the transformation of $\pm 1$ order modes from evanescent to propagating. According to the graphs in figure 3c and 3d, TM polarization allows for a clearer display of the Wood–Rayleigh resonances and sharper regime-transition peaks, forming a gap with a low reflectance level between these two points ($\lambda/\Lambda = 1.0$ and $\lambda/\Lambda = 1.46$).

Figure 4 demonstrates spatial distributions of electric and magnetic fields of the reflected and transmitted to the substrate radiation. The field distributions are calculated at extraordinary points.

Figure 4. Spatial distributions of the electric field (TE polarization case) and the magnetic field (TM polarization) of the reflected and transmitted to the substrate radiation for gratings at different $\lambda/\Lambda$ ratios and GST phases (A – amorphous, C – crystalline). The grating height is 70 nm. The deeper color corresponds to a more intense field.

Point $\lambda/\Lambda = 1.0$ corresponds to the first-order Wood–Rayleigh grating resonance; point $\lambda/\Lambda = 1.5$ (and 1.4 in TM case) corresponds to the edge of subwavelength regime (minimum of reflectance); and point $\lambda/\Lambda = 1.9$ corresponds to maximum of reflectance. The dependencies for TM polarization in figure 3(c, d) are similar for both phase states of the GST grating, and the magnetic field distributions
are also similar. For this reason, figure 4 provides field pictures only in the cases of the amorphous GST state for TM polarization. The electric field distributions for TE polarization in the amorphous and crystalline states of GST (figure 4, rows 1 and 2) also have similar patterns despite significantly different curve behaviors (see figure 3a, b).

There are several ways to interpret the results. If the diffraction grating is used for optical switching of the GST phase by external irradiation, the reflection spectra help identify the parameters when high or resonant absorption in GST occurs, and the field distributions provide a visual representation of the regions of energy concentration. Furthermore, the diffraction grating may be even used as an input port of a memory cell exploiting different levels of coupling efficiency that strongly depend on reflection levels (see, for example, figure 3a, b). Another variant is possible when the diffraction grating is used for enhancing the existing optical phase-switching mechanism by reducing the time and energy parameters via concentrating the EM field in certain regions of the grating.

In conclusion, we demonstrate one possible way of applying a structural design approach involving diffraction gratings with subwavelength or compared to the wavelength dimensions to the concept of a photonic non-volatile memory cell that utilizes the GST material with a switchable phase. This can be particularly helpful for designing memory cells with different mechanisms of the GST phase switching. Furthermore, the same approach may be used for designing multilevel memory cells, when, for example, the phases of each constituent element of the GST grating is switched separately. To this end, waveguide-grating structures may be considered as a conventional continuous waveguide and a discrete waveguide composed of a linear chain of nanoparticles [19]. In this case, the problem is an EM coupling between the modes of a continuous waveguide and the collective modes of a nanoparticle chain.

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