All-optical tuning of EIT-like dielectric metasurfaces by means of chalcogenide phase change materials

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Abstract: Electromagnetically induced transparency (EIT) is a pump-induced narrowband transparency window within an absorption line of the probe beam spectrum in an atomic system. In this paper we propose a way to bring together the all-dielectric metamaterials to have EIT-like effects and to optically tune the response by hybridizing them with a layer of a phase change material. We propose a design of the metamaterial based on Si nanoresonators that can support an EIT-like resonant response. On the top of the resonators we consider a thin layer of a chalcogenide phase change material, which we will use to tune the optical response. Our choice is Ge2Sb2Te5 (GST), since it has two stable phases at room temperature, namely amorphous and crystalline, between which it can be switched quickly, nonvolatively and reversibly, sustaining a large number of switching cycles. They differ in optical properties, while still having moderately low losses in telecom range. Since such dielectric resonators do not have non-radiative losses of metals around 1550nm, they can lead to a high-Q factor of the EIT-like response in this range. Firstly, we optimize the starting structure so that it gives an EIT-like response at 1550 nm when the GST layer is in the amorphous state. Our starting design uses glass as a substrate, but we also consider implementation in SOI technology. If we then switch the thin layer of GST to its crystalline phase, which has higher losses, the EIT-like response is red shifted, providing around 10:1 contrast at 1550nm. This reversible tuning can be done with an ns visible pulsed laser. We discuss the results of the simulation of the dielectric metasurface for different configurations and the tuning possibility.

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1. Introduction

Observation of a narrowband transparency window within a wide absorption line of the spectra in atomic physics is known as electromagnetically induced transparency (EIT) [1]. It is followed by dramatic dispersion and high-Q resonances which make it interesting for the slow-light effects [2], nonlinear effects’ enhancement [3], improvements in optical sensing etc. The need for chip-scale implementation of such effect has triggered research in EIT-like metamaterials that are designed to mimic it. This is typically done using the coupling between the so called bright resonator, broadband and excited directly by the light, and the dark resonator, that poorly couples to the light. When designed properly, the interference between these two resonators and the low radiative loss of the dark resonator could lead to very sharp, narrowband transparency windows. These resonances have an extremely steep phase change that leads to the decrease of the group slow-light effects [2], nonlinear effects’ enhancement [3], improvements in optical sensing etc. The need for chip-scale implementation of such effect has triggered research in EIT-like metamaterials that are designed to mimic it. This is typically done using the coupling between the so called bright resonator, broadband and excited directly by the light, and the dark resonator, that poorly couples to the light. When designed properly, the interference between these two resonators and the low radiative loss of the dark resonator could lead to very sharp, narrowband transparency windows. These resonances have an extremely steep phase change that leads to the decrease of the group
velocity, which was successfully demonstrated with EIT-like behavior with metal based metamaterials in GHz and THz range [4–9]. Unfortunately, in the optical region the limiting factor of metal-based EIT-like metamaterials are huge ohmic non-radiative losses of the dark resonator that set Q factor under 10. The potential solution is to use high refractive index dielectric materials instead of metals – they can still provide magnetic and electric dipole response [10–13], while having low non-radiative losses. Recently it has been experimentally shown that all-dielectric EIT-like metamaterials based on Si can lead to Q factor up to 130 in the near-infrared domain [14,15].

The next step towards novel applications of EIT-like devices would be the possibility to optically tune their response. Indeed one of the hottest topics in nanophotonics are the principles, design and fabrication of active subwavelength elements that can fast change amplitude or phase of transmission or reflection over nanoscale propagation lengths. For example, there have been attempts to control the spectrum, direction and divergence of light by using the active layers of liquid crystals, resulting in the switching times on the order of 100µs [16,17]. However, nowadays we need the compatibility with fast optical systems that work with ns pulses, and the fast low-power optically controlled switcher is still a challenge. A potential solution is the use of phase change materials (PCM) that can be quickly, nonvolatively, and reversibly switched between the two stable phases that differ in electrical and optical properties. If such a layer is put in contact with our designed structure, the changes in complex refractive index would produce a huge change in optical properties of the overall structure, thus allowing the manipulation of the incoming beam [18–21]. For these purposes the PCMs used are chalcogenide glasses that switch between crystalline and amorphous phase upon a heat stimulus. The most investigated and used one, Ge2Sb2Te5 (GST), has both phases stable at room temperature, and the recrystallization time less than 20ns, which is why it has been used for many years in rewritable optical discs and related phase-change memory applications [22,23]. Its switching can be optical, thermal or electrical, with switching repeatability as high as 106 cycles. GST has been applied in plasmonics to tune the response of metal-based metamaterials [24,25], 2D arrays of nanoholes [26,27] etc. On the other hand, metamaterials could be utilized to improve the switching performance; in [28] metamaterials’ resonances lower the power and shorten the time needed for the phase change to take place. There is, however, a limitation due to high diffusion between GST and metal layer during the heating [29], which is in general solved by the introduction of an additional protective buffer layer between them. Recently it has been shown that phase change degree of GST can be controlled via fs pulses leading to reconfigurable metasurfaces [30]. Moreover, in [31] it has been experimentally demonstrated that GST grating on SiO2 can provide contrast ratios up to 5:1 at visible/near-infrared wavelengths.

Here we propose an EIT-like metamaterial which is functionalized by an active layer of GST deposited above. We want to tune the optical response by changing the losses of the dark resonator. The starting structure is a multilayer of GST thin film that is deposited on 120nm layer of Si upon a glass substrate, or 120nm Si upon SiO2 on Si substrate (SOI configuration). This layer is then to be patterned according to EIT-like recipe: it should contain bright and dark resonators, for which we use simple dipole antenna resonators, and square-like rings, respectively. Since amorphous GST state has lower real and imaginary refractive index at 1.55 µm, we design our EIT-like feature supposing that GST is in this state. We further investigate how these resonances depend on the geometric features, and on the substrate employed. We also simulate the situation in which GST layer has been deposited after the EBL patterning, covering the whole structure. To be switched to crystalline state, GST needs to be heated above its crystallization temperature (Tcr~160°). Higher refractive index of crystalline state shifts these resonances, and higher losses widen them, so that the previous feature is destroyed, leading to high contrast ratio (CR) and modulation depth (MD) at 1.55 µm. For reamorphization of GST layer it needs to be heated by higher intensity beam above its melting point (Tmel~620°), and then quickly cooled down; since here it is in touch with very stable Si nanoresonators, we do not expect instability problems of diffusion and melting of the metamaterial layer, as experienced in metal-based PCM hybrid structures.
Finally, we perform transient thermal calculations to monitor this switching by a pump beam of the visible wavelength, where GST absorbs efficiently - a pump beam induces amorphization or crystallization, leading to the switching of the probe response at 1.55μm between EIT-like resonance, and transmission dip, respectively.

2. Structure and design

We have used Lumerical finite-difference time-domain (FDTD) Solutions package to simulate and optimize our structures. In Fig. 1(a) unit cell and the constituents of our metamaterial are shown, as well as GST refractive indices from [19]. We assume the structure to be infinite in x and y direction, with the periodicity p in both directions, and we apply periodic boundary conditions in these directions; along the z direction we apply a perfectly matched layer condition. The nanoresonators are made of Si of thickness t = 120nm, above which there is a thin layer of GST, tGST on the order of 15nm, and they are placed upon a semi-infinite glass substrate; in the inset of Fig. 1(a) the x-z cross section of the metamaterial is shown. The nanorod resonator supports a dipole-like low-Q collective mode when the incident light is parallel to its long axis, Fig. 1(b). Its parameters are the length L, and width W, and a metamaterial that consists only of these “bright mode” nanobars is designed with proper parameters so that it gives typical transmission minimum around 1.55μm (not shown here), which gives us starting values before the optimization: p and L should be around 1.05μm and 950nm, respectively. For the dark resonator we chose square-like ring resonator that cannot be excited directly by the incoming field, since there is no normal magnetic field component, Fig. 1(c); their parameters are the inner radius rin and the width Wr. This ring-based combination, when optimized, can lead to high-Q EIT-like response; simpler dielectric nanoparticles have their own strong magnetic and electric resonances, therefore in this geometry they would become excitable by the incoming field (they would stop being “dark”). The distances between two adjacent resonators are a in the same cell, and b from the adjacent cell. We chose the ranges for our parameters to be far from critical for the EBL patterning which is the subject of the current work. Since GST has been widely investigated and used as a thin layer in nowadays technology, we do not expect big problems during the fabrication that will include etching of the starting multilayer to the final structure of Fig. 1(a)-1(c). All-GST nanoresonators are also interesting for investigation; however, in our case the thicker layer of low-lossy GST would destroy a high-Q feature, and the all-optical control would be less uniform and more power-consuming.

Metamaterial analogue of EIT relies on the possibility of the structure to support a destructive interference between possible pathways of collective modes excitation, and in this way it is a classical analogue of quantum destructive interference that takes place in atomic systems with three levels, Fig. 1(d). In our case, the bright collective mode can be directly excited by the incoming light whose electric field is oriented along the rod (blue arrow in Fig. 1(d), path |0> → |1>). Magnetic field formed around such an excitation can consequently excite the dark mode, since it is now perpendicular the surface of the ring. The excited dark mode can couple back to the bright mode, providing the second, indirect path for its excitation (violet arrows in Fig. 1(d), path |0> → |1> → |2> → |1>). Under proper geometrical conditions these two pathways interfere destructively, and across the transmission dip, which is typical for the dipole-like resonance, a sharp, EIT-like transmission peak arises. Our metamaterial shows the EIT-like peak when the upper GST layer is in the amorphous state. If we then apply a pump beam in order to induce the temperature increase, the energy is prevalently absorbed in the GST layer above the ring, i.e. dark resonator. This layer will be therefore switched to the crystalline state; this changes the complex refractive index of the dark resonator, red-shifts the resonances and destroys the destructive interference, resulting in a dipole-like transmission minimum. EIT-like peak can be reversibly turned on by amorphization of the same layer. In the simulations we have used the refractive indices from [19], shown in Fig. 1(e-f), and in all simulations air is set as a surrounding medium.
3. Results and discussions

In the following we propose a way to all-optically tune the EIT-like peak. We employ the optimization algorithm to optimize the characteristic figures of merit (FOM) and we address the possibility of using a SOI sample. We then address the temperature and time dependence of this switching, which is to be experimentally induced by using a visible pump beam. Finally, we consider the case in which GST layer is deposited above whole metamaterial surface, after the patterning.

3.1. Optimization of the contrast ratio

We design our metamaterial so that it has EIT-like response at 1.55μm when the GST part of the resonators is in the amorphous state. This high transmission (and low group velocity) state can then be switched to a low transmission state, if the upper GST layer of the dark resonator is switched to the crystalline state. The figures of merits we use to define the efficiency of such a transmission switch are: the contrast ratio CR = T_{am}/T_{cr}, and modulation depth MD = T_{am}-T_{cr}, which are the ratio and the difference between the powers transmitted in the amorphous and crystalline state, respectively. To optimize these FOMs we use particle swarm algorithm, already implemented in Lumerical FDTD. We keep the thickness of the Si layer at 120nm, while for t_{GST} we suppose that it should be thin enough to be easily controlled by a moderately low power pump beam, but thick enough to provide for the resonance shift. Therefore we vary this parameter from 10nm to 30nm, supposing that it has been deposited before the patterning, so that there is no GST on the glass bottom, between the resonators. The optimization algorithm gives us the following parameters: \( p = 1046nm, \quad L = 963nm, \quad W = 156nm, \quad W_r = 110nm, \quad r_{in} = 154nm, \) and \( t_{GST} = 17nm, \) with the distances \( a = 223nm \) and \( b = \)
leading to CR of 10.5 and MD of 0.7936 at the desired wavelength, Fig. 2, and having Q~220. Since the position of the resonance is mainly defined by $p$, this parameter is critical in setting the wavelength, while other parameters control the Q factor. None of these values is critical for standard patterning. This is in agreement with the asymmetry issue arising from the fact that each nanosquare is being excited by the two opposite magnetic fields from two adjacent nanorods; if these excitations are equal ($a = b$), the overall magnetic field is zero, so there is no possibility to get EIT-like resonance [14].
In Fig. 3 we show the field distributions at the EIT-like resonance at 1.55μm in the amorphous state (top), and without this effect, in the crystalline state (bottom). At EIT-like peak there is no characteristic dipole-like distribution of the electric field – the bright collective mode does not resonate, Fig. 3(a). Instead, there is a large magnetic field in the nanosquare resonators, showing the indirect excitation of the dark mode, Fig. 3(b). If we then switch GST of the dark resonator to the crystalline state, we see no EIT-like distributions - we see a dipole-like mode distribution in the electric field, Fig. 3(c)-3(d). We can therefore confirm that we can switch off the EIT-like effect by inducing the optical phase change in the GST part of this resonator.

3.2. Influence of the substrate

Fig. 4. Influence of the SiO2 layer thickness when the metamaterial is produced in SOI technology. (a) Spectra dependence on $t_{SiO2}$ when GST is in the amorphous state. (b) Spectra dependence on $t_{SiO2}$ when GST is in the crystalline state. (c) Periodically changing transmission at 1.55μm as a function of $t_{SiO2}$. (d) Periodically changing CR spectra as a function of $t_{SiO2}$.

From the practical point of view, it is always desirable to implement the novel approaches into already existing reproducible and reliable technology. Here we investigate whether the SOI substrates can be employed to support such responses. We start from the Silicon on insulator substrate which has $t$ layer of Si upon $t_{SiO2}$ buried oxide, that lie on a semi-infinite Si substrate. We suppose that we have added a thin layer of GST, and then done the patterning. Here we have to be careful about the fact that our resonances can be suppressed or enhanced by constructive and destructive interference of the incident light reflected from the SiO2 layer [12]. Therefore we fix all of our optimized parameters from §3.1. and change $t_{SiO2}$ layer from 0 to 5000nm, in the 50nm steps, for the amorphous and crystalline GST, Fig. 4(a) and 4(b), respectively. For thinner, $t_{SiO2} \leq 500$nm layers coupling to the semi-infinite Si substrate is huge, and we do not observe any resonant behaviour. Therefore such thin SOI samples cannot be used as a starting structure for this wavelength. Then, for $t_{SiO2} \sim 1000$nm, the coupling is still
great, but we start to observe resonant behaviour. Starting from $t_{SiO_2}>1000\text{nm}$, we can get the EIT-feature in the amorphous state, but it is periodically enhanced and suppressed due to the interference. Indeed, if we plot the transmission maximum at the EIT-like peak as a function of $t_{SiO_2}$, Fig. 4(c), we see that the period equals to the half wavelength across the substrate. We then plot the same results for the crystalline state. In Fig. 4(d) we show the dependence of CR — as expected, it is as well periodically enhanced and suppressed. This behaviour suggests that any SOI structure with GST deposited layer could be patterned with optimized parameters so that it gives high CR and MD at a wanted wavelength. Moreover, CR can be even enhanced with optimal $t_{SiO_2}$: for the simple glass substrate (§3.1.) the optimized CR was around 12, while here we can get CR as high as 18.

3.3. Optical switching

GST layer in hybridized structures could be switched thermally, electrically or optically, the last being the fastest way, thus of the interest for our all-optical design. For the amorphization, the layer needs to be brought to a temperature higher than $T_{\text{mel}}$, and then quickly cooled down, preventing the slower process of recrystallization. This is conventionally done by a short and high intensity pulse in the visible range. Since we have a thin layer of GST, the fair expectation is that during the amorphization process Si in our resonators will also be brought to a very high temperature. Here we underline that one of the advantages in merging PCMs with Si-based dielectrics is exactly the fact that these materials are stable at high GST transition temperatures, so there is no need to use buffer layers to prevent diffusion and melting, as in metals [25,29]. However, the issue of the refractive index change of our resonators should be addressed, but it is out of the scope of the current work. For the crystallization to occur, the longer, low intensity optical pulse should be employed to bring the GST layer temperature above $T_{\text{cryst}}$ (but below $T_{\text{mel}}$). Here one should tackle the speed and power issues of the switching, since it is largely limited by the slow recrystallization times — it is desirable to be on the order of ns, while having the low total power. In [28] the trade-off between the short crystallization time and high power is solved by using the perfect absorber resonances of the metamaterial.

Here we address the dynamics of the optical switching of our metamaterial, by means of combined FDTD and DEVICE calculations from Lumerical. For the size of the array we follow the Q-dependence analysis outlined in [14]. Namely, we need to ensure that the number of unit cells is sufficiently big so that the coherence of our modes does not break due to the scattering from the edges of the structure. We therefore chose a 100 x 100 pattern of quadratic unit cells, for which the transmission of the probe beam would show a good enough Q-factor when GST is in the amorphous phase. This implies that the visible pump beam, which controls the surface of approximatively FWHM$^2\pi/4$, needs to be able to phase switch the GST layer in 100$^2$ unit cells. Figure 5(a). For this purpose we can see that FWHM$^2 > 100^2(4\pi^2/\pi)$, which gives us FWHM=120µm. In Fig. 5(b) we show the shorter wavelength part of the absorption spectra of our metamaterial when GST is in the crystalline phase. In agreement with the literature, we chose the input source at 660nm, where there is an increase of the absorption in our structure. Our FDTD simulation calculates the power absorbed by the unit cell when the incident beam is 1mW, and scale it by factor $1/(100^2)$, which approximatively gives the fraction of the power absorbed by one unit cell. This absorption serves us an input heating source in our thermal simulation, which embodies the same geometry and uses the values for thermal conductivity and heat capacity of GST from [25]. The transient simulation uses this heat source as a 50ns pulse for the amorphization, and 100ns for the crystallization, typically used for this material [19,25]. The next step is to scale the input source so that in the temperature of the top GST layer of the ring reaches the value critical for the phase change to take place. Our first calculations showed that the absorbed energy is always much more concentrated in the dark resonator, so that it reaches high temperatures $T_{\text{mel}}$ and $T_{\text{cryst}}$ much earlier than the layer over the rod. This lowers the overall power since we need to control only the temperature of the ring, to induce the phase change in its layer of GST, while GST layer over the rod stays always in the amorphous state.
We start from the optimized structure with GST layer in the amorphous state. For the crystallization to take place on the ring, we calculate that we need a 100ns pulse of $I = 0.0165$ mW/μm$^2$ (with the assumed FWHM). In Fig. 5(c) we shows that the ring’s GST layer reaches 720K, while the bar’s is mainly at the temperature much lower than this, therefore it will stay in the amorphous phase. The amorphization is more demanding process in terms of power, and we show that a 50ns pulse of $I = 0.0238$ mW/μm$^2$ can bring the ring’s GST to 893K, which is enough to be amorphized, Fig. 5(d). Since during the crystallization pulse bar’s GST layer stays in the amorphous state, during the reamophization high temperature regions on the bar will change the overall optical properties.

![Fig. 5](image)

**Fig. 5.** (a) Scheme of the all-optical tuning. (b) Shorter wavelength absorption spectra of the metamaterial. (c) Results of the transient simulation for the crystallization. (d) Results of the transient simulation for the amorphization.

At this point it should be added that high-n dielectric metasurfaces could be designed so that they have different electric and magnetic resonances in the visible domain, in which case it should dramatically decrease the power needed to induce the phase transition, as in the case of [28]. Moreover, the possibility to induce meta-stable phases between the two, by using fs pulses, should open more prospects in the tuning of such structures [30].

### 3.4. Influence of GST on the bottom

From the fabrication point of view, the EBL parameters need to be optimized before the patterning with the deposited GST layer is done. Perhaps our novel hybridizing of the all-dielectric metasurfaces with thin PCMs is more controllable when we perform typical EBL patterning of Si on glass or SOI, and then uniformly deposit a thin layer of GST above the whole structure. $xz$ cross section of such device is shown in Fig. 6(a). Here we again perform the simulations to get an EIT-like peak when GST is amorphous, supposing that we have successfully deposited $t_{\text{GST}} = 10\text{nm}$ on the top of the nanoresonators of the thickness $t_{\text{iSi}} = 120\text{nm}$ (we can expect less than ±1nm control of this thickness [32,33]). Such a metamaterial gives the transmission peak at 1.55 μm, when the parameters are: $p = 1030\text{nm}$, $L = 900\text{nm}$, $W = 160\text{nm}$, $W_r = 100\text{nm}$, and $r_{in} = 150\text{nm}$, Fig. 6(b). Since the effective volume of higher index environment increases if GST is also present at the bottom, the spectral response will be red-shifted with respect to §3.1, therefore we need smaller periodicities to bring the peak back to 1.55μm. Moreover, overall losses that are now higher, decrease Q factor. If we then try to
tune this peak, by using the absorption at 660nm (Fig. 6(c)) to crystallize GST, we see the intensity needed is higher than in §3.3, Fig. 6(d). Moreover, temperature is highly non-uniform, having huge regions at the bottom and at the top of the rod that have also reached T_{cryst}. We can therefore conclude that such metamaterials with GST deposited after the EBL patterning are less stable than the previously proposed ones. We believe that a design that gives more thermally uniform response could be obtained with using simpler geometries (e.g. nanorod metamaterial covered by GST for all-optical switch without EIT-like resonances).

Fig. 6. (a) Sketch of the structure in the case where GST layer is subsequently deposited after the EBL patterning. (b) Transmission spectra when GST is amorphous. (c) Absorption spectra when GST is amorphous. (d) Simulation of the crystallization.

4. Summary

In conclusion, we have proposed the all-optical, non-volatile, high CR and MD transmission switch based on Si nanoresonators activated by a thin layer of GST deposited above, and optimized to work at 1.55\,\mu\text{m}. Our proposal leads to the EIT-like transmission peak when the active GST layer is in the amorphous state, interesting for slow-light applications. The GST layer can be quickly, reversibly, and nonvolatively switched to the crystalline state, where the EIT-like effect is destroyed. Since the higher refractive index and absorption losses red shift and widen the spectra, our structure is optimized so that the transmission minimum in the crystalline state happens at the same wavelength as the maximum in the amorphous state, with CR above 10. We have then investigated how the implementation in SOI technology changes our resonances, as well as the influence of the GST layer on the bottom of the unit cell. We have then performed thermal transient simulations to find the properties of the pump laser that is to be used in the future experiments. Merging of all-dielectric resonators and GST increases the stability of the operation since we do not need additional buffer layers between them to prevent the diffusion and melting, as in metal-based metamaterials. We strongly believe that such a new concept could lead to great improvements in all-optical photonics.