Abstract We propose all-dielectric metasurfaces that can be actively re-configured using the phase-change material Ge\textsubscript{2}Sb\textsubscript{2}Te\textsubscript{5} (GST) alloy. With selectively controlled phase transitions on the composing GST elements, metasurfaces can be tailored to exhibit varied functionalities. Using phase-change GST rod as the basic building block, we have modelled metamolecules with tunable optical response when phase change occurs on select constituent GST rods. Tunable gradient metasurfaces can be realized with variable supercell period consisting of different patterns of the GST rods in their amorphous and crystalline states. Simulation results indicate a range of functions can be delivered, including multilevel signal modulating, near-field coupling of GST rods, and anomalous reflection angle controlling. This work opens up a new space in exploring active meta-devices with broader applications that cannot be achieved in their passive counterparts with permanent properties once fabricated.

Active dielectric metasurface based on phase-change medium

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1. Introduction

The development of flat and compact optical devices has drawn much interest owing to its potential applications in electromagnetic wave modulation. Much attention has been directed toward devices made of either metamaterials or metasurfaces consisting of ultrathin artificial subwavelength structures. Metamaterials have been shown to demonstrate many exotic optical properties, such as electromagnetically induced transparency (EIT) [1–4], optical Fano resonance [5–8], optical super absorber [9, 10], giant nonlinearity [11, 12], and optical negative refraction [13–15] among others [16]. However, because of the tremendous loss associated with the metal components embedded in these three-dimensional (3D) structures, metamaterials have little chance to be employed in applications where efficiency is a matter of concern. To this end, metasurfaces [17–19], the two-dimensional (2D) version of the metamaterial, where light is not required to have a deep penetration, have been used to show exceptional functionalities in manipulating various optical properties, such as flat lens [20, 21], meta-hologram [22, 23], and polarization control [18, 24]. While metasurfaces have demonstrated better performance in efficiency by comparison with the 3D metamaterials, the loss is still a significant concern because of the metal elements commonly used here [25, 26]. It is therefore desirable to do away with any metal altogether by applying the all-dielectric approach [27–30]. For example, using stacked silicon rods, zero-index low-loss metamaterial at optical frequency has been realized, and the modulation of the light emission from the quantum dots nearby this metamaterial has been demonstrated [30]. Also, low-loss EIT metasurface consisting of silicon nanoantenna for refractive index sensing is demonstrated recently [29]. The other limitation with the conventional metasurfaces is that their optical properties are typically permanent once the devices are fabricated. There is obviously a need to develop tunable all-dielectric “meta-devices” [31–33] where their

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optical responses can be actively controlled with external applied measures, such as force, heat, electric or magnetic field. One kind of material that can be conveniently applied to achieve such a unique feature is the phase-change media which exhibit dramatic differences in optical and electrical characteristics between its crystalline and amorphous states [34]. The phase transition can be induced by applying either heat [35], photon [36, 37], or electric energy [38–40] on the phase-change material. The reversibility between phase states can be realized by carefully modulating input energy pulse [41, 42]. Such phase-change materials have been widely used in commercial rewritable optical disks [36] and as media for storage cells in electronic phase-change memories [39, 40]. These properties can provide active modulation or switching when applied properly to metasurfaces. So far, most studies concerning phase-change materials only employ them as surrounding medium for metallic subwavelength structures by using their dielectric constant change to tune the plasmonic resonance for optical switching [43–46]. For example, by placing a metasurface on the phase-change medium, the Fano resonances on the metasurfaces can be tuned reversibly, resulting in a high-contrast optical signal modulation [43, 45]. These metamaterials still use metal to generate plasmonic resonances with phase-change medium acting as background, as a result, they are lossy. An interesting question naturally arises – whether phase change materials can be used in place of metal on metasurfaces. Among the many different phase-change materials, Ge$_2$Sb$_2$Te$_5$ (GST) alloy is known to have advantages of low optical loss in the near infrared (NIR) range and non-volatility, high stability and quick response [43, 47]. To this end, artificially structured GST presents an interesting opportunity. In this paper, we study the fundamental optical response of the GST system made into unit blocks from which metasurfaces are constructed with properties that are not only otherwise nonexistent in nature but also controllable, with the goal to demonstrate reconfigurable meta-devices in NIR utilizing its tunable optical properties as it undergoes phase transition. We first numerically analyze the optical resonant modes associated with the GST rod as an optical dipole antenna with different crystallization levels. Based on this, we then propose a metasurface composed of addressable meta-molecules with constituent GST rods. Near-field coupling between the GST rods within a meta-molecule can be tuned by modifying the phase state of these GST rods. Finally, we validate the concept of reconfigurable gradient metasurface capable of exhibiting different anomalous reflection angles by controlling the combination of GST rods with different geometries and phase states. Such an active metasurface opens up the potential for tunable meta-devices with broader applications that cannot be realized in their passive counterparts with permanent properties once they are made.

2. Optical properties of GST rod

Experimental and theoretical investigations of the optical constants/dielectric functions of GST have been previously reported [48, 49]. Figure 1a shows the schematic of a GST rod as a unit block which behaves as an antenna that couples with the incident electromagnetic wave. We use the ellipsometrically measured refractive indices as well as extinction coefficients of GST in amorphous and crystalline states. $n_x$ and $k_x$ are the refractive index and extinction coefficient of $\alpha$-GST, $n_c$ and $k_c$ are those of $c$-GST, respectively [43]. Transmission spectra of the $\alpha$-GST (c) and $c$-GST rod arrays (d) of different length $L$ (e) Electric field enhancement and (f) z-direction electric field distribution of the $\alpha$-GST rod with $L = 450$ nm, where the three-dimensional axes are shown in (a).

Figure 1 Phase-change rod. (a) Schematic of the GST rod on freestanding SiN$_x$ thin film (unit cell) $P_x = P_y = 1000$nm, $W = 250$nm, $H_a = 50$nm, $H_b = 50$nm. The rod length $L$ is varied from 250 nm to 950 nm. (b) Optical constants of GST in amorphous and crystalline states. $n_x$ and $k_x$ are the refractive index and extinction coefficient of $\alpha$-GST, $n_c$ and $k_c$ are those of $c$-GST, respectively [43]. Transmission spectra of the $\alpha$-GST (c) and $c$-GST rod arrays (d) of different length $L$. (e) Electric field enhancement and (f) z-direction electric field distribution of the $\alpha$-GST rod with $L = 450$ nm, where the three-dimensional axes are shown in (a).
optical transmission spectra of a $\alpha$-GST rod with various lengths $L$ are shown in Figure 1c. When the incident polarization is parallel to the long axis of the rod, an obvious resonant feature can be found in each spectrum. The resonant wavelength of the rod is red-shifted with the increase of $L$. This relation is in good agreement with the theoretical prediction on the resonant properties of dielectric resonator, which can be described by: $p(\lambda/\alpha) \approx 2\pi L$, where $p$ is a positive integer, and $\alpha$ is the refractive index of GST at the resonance wavelength [51, 52]. We have analyzed the near-field distributions of different resonant modes arisen from the oscillation of the induced displacement currents in the GST rod. Figures 1e and 1f are the simulation results for the case of $\alpha$-GST antenna with $L = 450$ nm. The field distribution in Figure 1e shows the typical characteristics of electric dipolar resonance of the GST rod at the resonant wavelength $\lambda = 1235$ nm, where the field is strongly localized near the short edges (top and bottom ends). The enhancement of electric field can be as high as $\sim$ 10-fold relative to the incident field. In contrast, the resonant dip of c-GST rod is red-shifted in comparison with that of $\alpha$-GST rod of equal length. This result is associated to the increment of refractive index $n$ of GST after phase transition from amorphous to crystalline state which is similar to what has been shown by Mie scattering theory that the optical resonance of a dielectric nanosphere also red-shifts with the increasing refractive index $n$ of the material.

The optical/electrical multi-level states is an important characteristic of GST [54]. By controlling the applied energy on the GST rod, partial crystalline state due to the formation of nucleation in amorphous GST can be realized [53, 54]. The optical resonances of phase-change metasurfaces can thus be gradually tuned by employing this method. Among the several effective-medium theories developed for the description of the optical constants/dielectric functions of heterogeneous medium [55, 56], Lorentz-Lorenz relation [57] is one of the best candidates that has been successfully applied in the simulation of the Au nanodisks/GST thin film hybrid system in which the GST thin film is in different crystallization ratio [44]. Figure 2 shows the transmission spectra of a phase-change GST rod (length: 850 nm) with a crystallization fraction of 0% ($\alpha$-GST), 25%, 50%, 75%, and 100% (c-GST). The effective dielectric constant of the GST material in different crystallization conditions can be approximated using the Lorentz-Lorenz relation,

$$\frac{\varepsilon_{\text{CGST}}(\lambda) - 1}{\varepsilon_{\text{CGST}}(\lambda) + 2} = m \times \frac{\varepsilon_{\text{CGST}}(\lambda) - 1}{\varepsilon_{\text{CGST}}(\lambda) + 2} + (1 - m) \times \frac{\varepsilon_{\text{AGST}}(\lambda) - 1}{\varepsilon_{\text{AGST}}(\lambda) + 2}$$

where $\varepsilon_{\text{CGST}}(\lambda)$ and $\varepsilon_{\text{AGST}}(\lambda)$ are the wavelength ($\lambda$)-dependent dielectric constants of GST in crystalline and amorphous state, respectively, and $m$ is the crystallization fraction of the GST, ranging from 0 to 1. The electric dipole resonance of the GST rod is shifted toward longer wavelength with the increase of $m$. As can be seen in Figure S1 in supporting information, which is the change of the transmission versus wavelength under different crystallization ratio, by controlling crystallization ratio, multi-level optical signal modulation at a specific wavelength can be achieved. For example, five transmission levels can be clearly observed at $\lambda = 1310$ nm and $\lambda = 1550$ nm (see Table 1).

3. Tuning the EIT resonance on phase-change metamolecule by selective modification

Optical properties of metamolecules that are created artificially can be engineered through the design of geometrical parameters of their constituent “meta-atoms” inside [58–61]. Here we demonstrate through numerical simulation that properties of a metamolecule can be tailored actively by manipulating the phase states of its constituent GST rods that work as “meta-atoms”.

![Figure 2](image-url) Tuning of the transmission spectrum of GST rod array with the control of its crystallization fraction. Transmission spectra of GST rod with different crystallization fraction. By changing the crystallization fraction of GST rod, the resonance wavelength can be gradually tuned. Five transmission levels can be clearly observed at 1310 nm and 1550 nm.

Table 1 Transmission coefficients of GST rod array with different crystallization fraction at $\lambda = 1310$ nm and $\lambda = 1550$ nm

<table>
<thead>
<tr>
<th>Phase state</th>
<th>$\alpha$-GST</th>
<th>25% Crystal</th>
<th>50% Crystal</th>
<th>75% Crystal</th>
<th>c-GST</th>
</tr>
</thead>
<tbody>
<tr>
<td>Transmission at 1310 nm (%)</td>
<td>20.15</td>
<td>37.71</td>
<td>50.51</td>
<td>58.9</td>
<td>64.15</td>
</tr>
<tr>
<td>Transmission at 1550 nm (%)</td>
<td>56.25</td>
<td>43.85</td>
<td>29.35</td>
<td>16.45</td>
<td>10.33</td>
</tr>
</tbody>
</table>

Figure 3 Designation of the dolmen metamolecule with different composition of rod phase states that mimics the denomination principle used in the organic chemistry.

Figure 4 Active control of the Fano resonance by the phase-change dolmen metamolecule. (a) Geometrical parameters of the dolmen metamolecule. \( P_x = P_y = 1000 \text{ nm}, \ L_b = 650 \text{ nm}, \ L_d = 420 \text{ nm}, \ W_b = W_d = 300 \text{ nm}, \ H_b = 70 \text{ nm}, \ G_b = 150 \text{ nm}, \ H_d = 150 \text{ nm}, \ H_S = 50 \text{ nm}. \) (b) Transmission spectra of \( \alpha \)-dolmen, 1-transformed-dolmen, and 2-transformed-dolmen metamolecules with purple and pink indicating amorphous and crystalline state, respectively. (c) Electric field intensity and (d) z-component electric field strength around the \( \alpha \)-dolmen metamolecule at its EIT-like resonance, where the z-axis is denoted in (a).

When the phase state in one of the GST rods inside the metamolecule is modified, the optical resonance of the metasurface changes dramatically. The middle and bottom panels in Figure 4b show the transmission spectra of the 1-transformed-dolmen and 2-transformed-dolmen, respectively. The optical spectrum is significantly changed when the phase state of any rod in the metamolecule is modified. In the case of 1-transformed-dolmen, the transmission spectrum exhibits a similar EIT-like profile as that of \( \alpha \)-dolmen, but the resonant features are red-shifted and relatively broader. In order to clarify the impact of phase state of each rod to the resonant modes, the optical responses of the \( \alpha \)-GST and 1-transformed-GST rod pair are simulated and the results are shown in Figure S4. The incident light is illuminated on the metamolecule with a tilted angle of 35° to excite the quadrupole mode in the metamolecule [4]. It can be seen in Figure S4b that the resonant dip associated with the quadrupole mode of the 1-transformed-GST rod pair is broader than that of the \( \alpha \)-GST rod pair. This result can be attributed to the increased extinction coefficient of the GST rod that is in the crystalline state. Because the EIT-like spectral profile of dolmen metamolecule is the result of interference between the excitation pathways of dipole and quadrupole modes inside it [2], the modification of quadrupole resonance induces apparent variation in the spectral profile. Therefore, the resonant profile of 1-transformed-dolmen becomes broader than that of \( \alpha \)-dolmen. In the case of 2-transformed-dolmen, the EIT-like resonance disappears, leaving only the dipole resonance.
Transmission coefficients of dolmen meta-molecule arrays with different modification conditions at $\lambda = 1250 \text{ nm}$

<table>
<thead>
<tr>
<th>Phase state</th>
<th>Transmission (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha$-dolmen</td>
<td>72.59</td>
</tr>
<tr>
<td>1-transformed dolmen</td>
<td>56.88</td>
</tr>
<tr>
<td>2-transformed dolmen</td>
<td>49.42</td>
</tr>
<tr>
<td>1,2-transformed dolmen</td>
<td>39.33</td>
</tr>
<tr>
<td>1,3-transformed dolmen</td>
<td>43.94</td>
</tr>
<tr>
<td>1,2,3-transformed dolmen</td>
<td>30.24</td>
</tr>
</tbody>
</table>

The electric field distribution at the transmission peak ($\lambda = 1430 \text{ nm}$) of the EIT-like resonance for the 1-transformed-dolmen in Figure S6c shows antisymmetric electric fields around the two vertical rods, indicating excitation of the quadrupole mode. The out-of-phase electric dipole oscillation in the rods is attributed to the asymmetry of the phase states in the vertical rods that results in phase difference between the resonances in the two rods under normal incident excitation. The EIT-like resonance observed is thus related to the interference between the “bonding” and “anti-bonding” modes [59, 63] associated with the two GST rods in different phase states.

### 4. Tuning the anomalous reflection on phase-change metasurface

In addition to the control of optical resonance, selective modification of the phase-states of GST rods can also be applied to the application of wave-front modulation by the metasurface composed of such phase-change GST rods. Figure 5 illustrates the construction and switching mechanism of the proposed phase-change gradient-index metasurface operating at 1550 nm. The phase-change rods are used as the basic building block for controlling the light phase and intensity of the so-called anomalous reflection induced by metasurface [64] by tuning their phase state and geometry to construct the needed gradient indices on

The reflective metasurface consists of an array of GST nanorods with different phase states and a continuous Au mirror separated by a spacer layer. Under the illumination of a normal incidence (1550 nm), the metasurface can switch its reflection angle by modulating the phase state of each GST nanorod.
Design of tunable gradient metasurface. (a) Schematic diagram of a basic unit cell consisting of a GST nanorod (length \( L \), width \( W \), and height 80nm) on top of a 40 nm ZnS-SiO\(_2\) spacer and gold substrate. (b-c) Phase of the reflected light as the function of width \( W \) and length \( L \) of amorphous and crystalline GST nanorods at a wavelength of 1550nm. (d-e) Reflection phase and relative intensity of two selected GST nanorods with width and length of (260nm, 420nm) & (280nm, 510nm).

Figure 6  Design of tunable gradient metasurface. (a) Schematic diagram of a basic unit cell consisting of a GST nanorod (length \( L \), width \( W \), and height 80nm) on top of a 40 nm ZnS-SiO\(_2\) spacer and gold substrate. (b-c) Phase of the reflected light as the function of width \( W \) and length \( L \) of amorphous and crystalline GST nanorods at a wavelength of 1550nm. (d-e) Reflection phase and relative intensity of two selected GST nanorods with width and length of (260nm, 420nm) & (280nm, 510nm).

The function of \( L \) and \( W \) at the incident wavelength of 1550 nm. The polarization of incident light is parallel to the long axis of GST rods. Each GST rod here works as a dipole antenna capable of modulating both the amplitude and phase of the reflected wave. Optical phase modulation as large as \( 2\pi \) by tuning \( L \) and \( W \) can be achieved. Figures 6d and 6e show the optical phase response and reflection of GST rods with the dimensions of \( 420 \times 260 \times 80 \text{nm}^3 \) (dotted line) and \( 510 \times 280 \times 80 \text{nm}^3 \) (solid line) in crystalline (red line) and amorphous states (blue line), respectively. The abrupt optical phase shifts occur at dipole resonances. When GST rods are all in crystalline state, resonances are far away from 1550 nm and the optical phase shift varies slowly with the wavelength. In contrast, the dipole resonances of \( \alpha \)-GST rods are much closer to 1550 nm and their optical phase shifts are far more sensitive to wavelength change.

These GST rods in different phase states can be arranged to form the so-called supercells from which a tunable phase-change metasurface can be designed based on the generalized Snell’s law [18],

\[
\sin \theta_r - \sin \theta_i = \frac{\lambda}{2\pi} \frac{d\phi}{dy},
\]

where the reflection angle \( \theta_r \) and incident angle \( \theta_i \) are related by the phase gradient \( d\phi/dy \) along the \( y \)-direction. In the case of normal incidence (\( \theta_i = 0^\circ \)) and \( 2\pi \) optical phase change over the period of a supercell \( L_s \), \( d\phi/dy = 2\pi/L_s \) [66], and the reflection angle can be simply determined by \( L_s \),

\[
\theta_r = \sin^{-1} \left( \frac{\lambda}{L_s} \right).
\]

Figure 7 illustrates three designs of the tunable gradient metasurfaces, each with different supercell period. Figure 7a shows a supercell design with twelve \( \alpha \)-GST rods of two different geometries, the period of such a supercell is much larger than the incident wavelength and can be considered as infinitely large in practical sense. Changing the phase state of 6 rods into amorphous state as shown in Figure 7b, we arrive at a metasurface with the supercell period of 2400 nm. In a different combination, eight amorphous and four \( c \)-GST rods produce a supercell with the period of 4800nm. Obviously, there are other configurations that can be obtained with the active control of the phase change on each GST rod, and the result is abundant collection of interesting optical responses yielded from a single tunable metasurface. For example, the anomalous reflection for a normal incident light at 1550 nm for the three cases described above is clearly directed onto different angles of \( 0^\circ \), \( -40^\circ \) and \( -20^\circ \) as shown in Figure 8a. This numerical result is in excellent agreement with Equation (3). As expected, when the supercell period is large relative to the incident wavelength and can be approximated as infinite, the metasurface reflects the normal incident wave back at the same normal angle of \( 0^\circ \). This is also confirmed with the reflection wave-front being parallel to the metasurface plane as shown in Figure 8b. The wave-fronts for the other
two cases with the reflection angles of -40° and -20° are shown in Figures 8c and 8d. The simulation results are in good agreement with Equation (3). There are, however, some small unintended reflection peaks at 20° or 40° which we have not been able to completely suppress due to grating diffractions by the supercells.

To realize the selective modification technique on the proposed phase-change metasurface, several matured techniques used in phase-change-material-based technologies can be adopted. One of the possible methods based on phase-change electronic memory is plotted in Figure 9. The meta-atoms of the phase-change metasurface are made on the TiN electrodes (for converting the electronic energy to thermal energy) which are connected with the conducting wire. By applying electronic pulse on the specific meta-atoms, the phase state of the treated meta-atoms can be changed, resulting in the selective modification on the metasurface-based device. Other possible methods can be the conductive-AFM [38], laser-direct writing [67–69], and so on.
Figure 9 Schematics for realization of the selective modification of phase-change metasurface. The GST rods of the metasurface are deposited on TiN electrode (shown in gold color), and their phase states can be changed by applying electric current pulses through the conductive wire.

5. Conclusion and outlook

In conclusion, using numerical simulation we have demonstrated that the all-dielectric phase-change material GST can be used to obtain reconfigurable metasurfaces with functional diversity for light modulation. The switchable electric dipole resonance of phase-change rods are presented. In addition to phase transitions between amorphous and crystalline state, partial crystallization in GST can also be used to increase the tuning range and resolution of the metasurfaces for more complex light modulation. Using GST rod as the basic building block, we have designed a single metasurface that is capable of exhibiting tunable optical response when selected GST rods underwent phase change. Such a tunable, all-dielectric metasurface offers superior properties and performance over the conventional metal metasurfaces that are known to be inherently inefficient and untunable. This design work is intended to shed light on the use of phase-change GST for active metasurfaces and stimulate future experimental demonstration of such devices that go far beyond the conventional metasurfaces in terms of functionality.

Supporting Information

Additional supporting information may be found in the online version of this article at the publisher's website.

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References


Key words: reconfigurable metasurface, metamaterials, beam steering, Fano resonances, phase-change material.