Evolutionary Optimization of Graphene-Metal Metasurfaces for Tunable Broadband Terahertz Absorption

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Abstract—Tunable THz absorbers based on graphene frequency selective surfaces (FSSs) are designed using well established evolutionary optimization techniques. Random hill climbing (RHC) algorithm is applied to find the design with the broadest bandwidth. The effects of three factors including the substrate loss, structuring the substrate and using double layer patches, are examined. The optimum structure with broadest operation bandwidth consists of a perforated lossy substrate with a single layer patch and offers 1.95 THz absorption bandwidth around 2 THz central frequency leading to 100% fractional bandwidth.

Index Terms—Terahertz, absorber, tunable, graphene, frequency selective surface, broadband, random hill climbing optimization.

I. INTRODUCTION

Terahertz absorbers are currently the focus of extensive research efforts owing to their applications in various fields such as stealth technology [1], imaging [2] and sensing [3]. A FSS absorber is a periodic structure consisting of a substrate sandwiched between a ground plane and a patch layer [4]. The ground plane, which is mainly a metallic layer, prevents transmission of energy through the absorber. Consequently, the incident energy is captured in the structure at resonant frequencies and is dissipated through propagation in a lossy structure [4].

The strong desire for dynamic tuning of FSS absorbers has instigated investigation and proposal of several techniques to realize such absorbers. Some frequent examples are FSS based on varactor diodes [5], liquid crystals [6] and microelectromechanical systems (MEMS) switches [7]. However, these methods face with yet unresolved challenges at THz frequencies because of difficulties in integration, miniaturization, and biasing [8]. Graphene is a well-known potential candidate to overcome these limitations [8]–[11].

Graphene is a one-atom thick carbon layer which consists of carbon atoms arranged in a chicken-wire-like structure [12]. Discovered in 2004 [13], this material has a tunable conductance which can be controlled by electrostatic or magnetostatic field or by chemical modification [14]. This promising property of graphene resulted in the emergence of graphene-based THz absorbers, which are reported in several previously published studies [15]–[20].

In this letter, an evolutionary optimization algorithm is proposed to find the optimal THz absorber with tunable performance. This study has been extensively accomplished for microwave absorbers based on metallic patches [4]. However, to the best of our knowledge, there is no report on the evolutionary optimization of graphene THz absorbers. The combination of metal and graphene in the patch layer results in new challenges in the optimization process which are investigated in this work. Furthermore, the effect of three factors

are also studied: 1) the loss of the substrate, 2) structuring the substrate, and 3) single/double layer patches. The following section explains the design procedure in detail. Subsequently, section III outlines the results of the optimizations and finally, section IV concludes the letter.

II. DESIGN

Design process of a FSS absorber aims at the determination of substrate properties, patch configuration and array periodicity to achieve the optimal performance [21]. In this work, the frequency regime is fixed to the low THz. In addition, the height of the substrate and the periodicity of the array in both x (P_x) and y (P_y) directions are assumed to be 20 and 80 μm , respectively, and fixed during the whole optimizations.

Random initialized hill climbing algorithm (RHC) is chosen here to design the shape and material of the patch layer, due to the interesting properties outperforming many of the existing stochastic optimization methods for FSS design [21]. The details of this algorithm are presented in section II. B. The tunability of the absorber operation is obtained through introduction of graphene inclusions in the patch geometry. As proposed in [8], this tunability can be achieved by controlling the conductance through an electrostatic bias field, which is applied normal to the surface. More details on this feature of graphene are presented in section II. A.

Besides a single layer FSS structure, double layer configuration is also investigated. In structures with single layer patch, a DC bias voltage is applied between the patch and the ground plane in order to provide the electrostatic bias field, while in structures with double layer patch, the second layer can function as a gate instead of the ground plane. As a result of smaller distance between the gates in the latter case in comparison to the former one, a considerable reduction in the required bias voltage is achieved [8]. Choosing a very thin substrate may similarly be helpful for this purpose. However, bringing the ground plane very close to the patch strongly affects the FSS performance [8].

Two distinct materials are selected for the substrate, silicon dioxide with a lossless relative permittivity $\epsilon_r = 4$ [9], and a lossy polymer with the relative permittivity $\epsilon_r = 3.5 + 0.2j$ [17]. In addition to the usual homogeneous substrate, the effect of perforating the substrate, as a method for engineering its properties [4], is also examined. The optimum radius of the hole is determined by the optimization algorithm. Moreover, normal incidence is considered during all electromagnetic analyses.

A. Graphene Model

A graphene sheet is modeled by its tunable surface conductivity [14]. In the absence of spatial dispersion and magnetostatic bias field, one can model the conductivity by a scalar parameter [14]. Here, the spatial dispersion effect is negligible [22] and only the electrostatic bias is used to control the

Fig. 1. The surface conductivity of graphene. The more bias voltage is applied, the more conductive the graphene surface will be. This dependency is stronger at low terahertz frequencies (0.1- 4 THz).

graphene conductivity. Therefore, the surface conductivity is determined by [14]:

$$\sigma(\omega, \mu(\mathbf{E}_0), T) = \frac{je^2(\omega - j2\Gamma)}{\pi\hbar^2} \left\{ \frac{1}{(\omega - j2\Gamma)^2} \int_0^\infty \varepsilon \left(\frac{\partial f_d(\varepsilon)}{\partial \varepsilon} - \frac{\partial f_d(-\varepsilon)}{\partial \varepsilon} \right) d\varepsilon - \int_0^\infty \frac{f_d(-\varepsilon) - f_d(\varepsilon)}{(\omega - j2\Gamma)^2 - 4\left(\frac{\varepsilon}{\hbar}\right)^2} d\varepsilon \right\} \quad (1)$$

$$f_d(\varepsilon) = \frac{1}{1 + e^{(\varepsilon - |\mu_c|)/k_B T}} \quad (2)$$

where ω is the frequency and Γ is a phenomenological electron scattering rate which is assumed to be independent of the energy ε . In addition, T , $-e$, $\hbar = h/2\pi$, $f_d(\varepsilon)$, and k_B stand for the temperature, the electron charge, the reduced Plank's constant, the Fermi-Dirac distribution (2), and the Boltzmann's constant, respectively. μ_c is also the chemical potential which is dependent on electrostatic bias field ($\mathbf{E}_0$). The phenomenological scattering rate can be written as $(1/2\tau)$ [23], where τ represents the phenomenological scattering time equal to 0.34 ps [24], [25]. T is considered to be equal to the room temperature (300 K) and the regime of low field operation is assumed, which in turn justifies neglecting the nonlinear effects in graphene. The variation of surface conductivity in terms of frequency for different values of electrostatic bias field is shown in Fig. 1. It is observed that the graphene conductivity increases with the increase in the applied bias voltage. This property serves as a simple tuning mechanism based on electrostatic gating. Besides, the graphene nanoscale and planar structure is proper for miniaturization and integration especially for THz applications. To model graphene in HFSS [26], surface impedance ($Z_s = 1/\sigma$) is assigned to the graphene sheet as a boundary condition [8], [23], [27].

B. Optimization

The surface of the unit cell is divided into 8×8 pixels (Fig. 2a). RHC algorithm uses an input bit string (binary code), where each bit determines the material assigned to the corresponding pixel. Presence and absence of a presumed

Fig. 2. a) The unit cell of the FSS absorber. Its surface is divided into 8×8 pixels. b) There are three locations (pixels marked by circles, the ones marked by triangles and the gray pixels) each of which must contain at least one bias element.

material at each pixel is represented by 1 and 0, respectively. As mentioned above, for the sake of tunability, graphene is considered as a material in the patch layer. However, combination of graphene and other conventional conductors, like metals, increases the degrees of freedom in the design process. This in turn enables obtaining better optimum performances which are not feasible in a complete graphene based FSS. Therefore, four options are provided for a single pixel. They are gold, graphene with $\mu_c = 0.775$ eV ($E_0 = 4$ V/nm) which is tuned using the bias voltage, graphene with the same chemical potential which is fixed by chemical doping and air. A two-bit string is considered to determine the material type. More accurately, {00}, {11}, {10} and {01} represent gold, biased graphene, doped (unbiased) graphene and air, respectively. Finite conductivity as a boundary condition in HFSS is used to model the gold patches.

Mirror symmetries with respect to x and y axis as well as the diagonal symmetry is considered in the optimization (Fig. 2a). As a result, the electromagnetic response of the design will be independent of polarization under normal incidence [15]. Moreover, the whole patch configuration is determined once one eighth of the unit cell is known.

To apply bias voltage throughout the whole FSS surface, pixels to which biased graphene is assigned need to be electrically connected [8], [15]. The connection between these pixels may also be realized through gold inclusions. Consequently, a bias chain is obtained, which must be isolated from unbiased graphene pixels. One may think of shrinking the unbiased graphene pixels in order to prevent their connection to adjacent biased pixels. However, such a tiny margin hardly provides a safe isolation. Thus, the condition of 'no shared side with biased pixels' is imposed to unbiased graphene pixels.

To recognize the designs, in which correct connection between bias elements and isolation from unbiased pixels are foreseen, the following algorithm is followed:

- If there is no {11} pixel, the design is correct.
- If the design contains {11} pixels:
 - 1) The presence of at least one {00} or {11} is essential at the specified locations in Fig. 2b which are connecting gates to other pixels by symmetry and periodicity.
 - 2) There must be at least one {11} or {00} pixel adjacent to a {11} pixel, otherwise it is isolated.

A depth-first search (DFS) algorithm is used in this step to register all connected pixels to the very first {11} pixel in the bit string and if any {11} pixel remains separated from this chain after the search, the connection is lost.

- 3) Structures with {10} pixel adjacent to the bias chain are rejected.
- 4) The {00} pixels which met the first condition must be checked whether they are connected to the registered bias chain. If not, the connection is lost and the design is discarded.

Twelve optimizations with specific assumptions are carried out in this study. Two groups of designs need a detailed explanation:

1) *Designs with double layer Patch*: Both layers have the same pattern and two different gaps between the patch layers are examined, 1.68 μm and 0.2 μm .

2) *Designs with Structured Substrate*: To structure the substrate, a hole is drilled at its center. The optimum radius of the hole is chosen by the optimization algorithm from discrete values between 4 μm and 32 μm with a step equal to 4 μm . Thus, three additional bits are needed to represent these eight radii in the bit strings. The height of the hole is set to 18 μm to consider for a thin layer of the substrate which mechanically supports the patch layer.

III. RESULTS

The RHC algorithm stops when it reaches a maximum number of evaluations (1000 for the structures with homogeneous substrates and 1100 for the ones with perforated substrates). The optimum results are presented in Fig. 3.

The broadest bandwidth (1.95 THz) is achieved by the optimum design, in which the substrate is the perforated lossy polymer and the patch is single layer (Fig. 3m). The bit string of this design is {01 01 11 01 11 00 11 01 11 01 111}. The last three bits stand for radius equal to 32 μm . Different absorption levels are obtained by applying various bias voltages to the biased graphene pixels of this design (Fig. 4).

IV. CONCLUSION

Evolutionary optimization of graphene-metal metasurfaces is introduced as a promising approach to achieve designs meeting an application requirement. In this work, random hill climbing algorithm is used to find a graphene-based FSS design for tunable broadband THz absorption. Tunability of the designs is realized by including graphene patches which results in a simple tuning mechanism. Lossless and lossy substrates are examined as well as single and double layer patches. The broadest bandwidth of 1.95 THz is obtained by the optimum design of a structure which has a perforated lossy substrate and a single layer patch.

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Fig. 3. Dark gray, bright gray and gold pixels represent biased graphene, unbiased graphene and gold, respectively. Schematics of the optimum designs of the structures with homogeneous silicon dioxide substrates: (a) single layer patch, double layer patch with (b) $d=1.68 \mu\text{m}$ and (c) $d=0.2 \mu\text{m}$. (d) The absorption versus frequency of the corresponding optimized structures (about 1.5, 1.55 and 0.95 THz bandwidth for the schematics of (a), (b) and (d), respectively). Schematics of the optimum designs of the structures with homogeneous lossy polymer substrates: (e) single layer patch, double layer patch with (f) $d=1.68 \mu\text{m}$ and (g) $d=0.2 \mu\text{m}$. (h) The absorption versus frequency of the corresponding optimized structures (about 1.65, 1.6 and 1.1 THz bandwidth for the schematics of (e), (f) and (g), respectively). Schematics of the optimum designs of the structures with perforated silicon dioxide substrates: (i) single layer patch, double layer patch with (j) $d=1.68 \mu\text{m}$ and (k) $d=0.2 \mu\text{m}$. (l) The absorption versus frequency of the corresponding optimized structures (about 1.7, 1.85 and 1.5 THz bandwidth for the schematics of (i), (j) and (k), respectively). Schematics of the optimum designs of the structures with perforated lossy polymer substrates: (m) single layer patch, double layer patch with (n) $d=1.68 \mu\text{m}$ and (o) $d=0.2 \mu\text{m}$. (p) The absorption versus frequency of the corresponding optimized structures (about 1.95, 1.85 and 1.45 THz bandwidth for the schematics of (m), (n) and (o), respectively).

Fig. 4. Different absorption levels are obtained by applying various bias voltages to the the optimum design of the structure which has a perforated lossy polymer substrate and a single layer patch. This optimum design has the broadest bandwidth of 1.95 THz when $\mu_c = 0.775 \text{ eV}$.

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