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Using High- k VPP Modes in Grating-Coupled Graphene-Based Hyperbolic Metamaterial for Tunable Sensor Design

A.K.M. Hasibul Hoque, Md Zahurul Islam, Mashnoon Alam Sakib, and Ying Tsui

Abstract—Volume plasmon polariton (VPP), a high- k mode that arises due to the coupling between two even modes of adjacent layers of an hyperbolic metamaterial (HMM) configuration, is very difficult to be excited by using prism coupling technique due to huge wave-vector mismatch. In this work, we present a graphene-based HMM structure integrated with metal grating to facilitate excitation of VPP modes. A graphene HMM is composed of multilayer graphene super-lattice similar to metal-dielectric super-lattice structure. We report the analytical formulation of the dispersion relation and numerical analysis of the characteristics of the excited VPP modes for the proposed structure in Terahertz frequency region. The best achieved imaging resolution (spatial) of our proposed structure is 15 nm when used as an infra-red imaging platform. As a sensing platform, a maximum sensitivity of 11,050 nm/RIU is achieved for this configuration. The tunability of the resonance wavelength with respect to the structural parameters of the device is also studied and confirmed. Such promising findings are expected to make the proposed structure with integrated excitation coupler a potential candidate for tunable sensor design for different nanophotonic applications, including imaging, and, biomedical and chemical sensing applications.

Index Terms—Graphene-based Hyperbolic Metamaterial, Volume Plasmon Polariton, Plasmonic Sensor, Tunable Sensor Design

I. INTRODUCTION

GRAPHENE, a two-dimensional allotrope of carbon arranged in a honeycomb lattice [1], has attracted a lot of attention in the area of photonic research due to its extraordinary tunable electronic and optical properties. Electromagnetic waves can strongly interact with graphene electrons, especially in the Terahertz region, leading to the charged-oscillation of the carrier and creation of graphene plasmons [2,3]. The characteristics of graphene plasmons are different from its noble-metal counterpart due to its strong confinement [4,5], low loss [4], tunability [5,6] etc. For these exceptional properties of graphene plasmons, graphene has been studied extensively for its applications in many areas, such as, photo detection [7], optical modulation [8], sensing [9,10], imaging [11] and tunable sensor design [12, 13]. Moreover, graphene-based super lattices or metamaterials also show some exotic

properties [14–16], which may expedite the commercialization of graphene-based devices.

Metamaterials are artificial sub-wavelength structures comprising of multiple materials. Metamaterials manifest unusual electromagnetic properties, such as, negative refraction [17], super-lensing [18] and electromagnetically-induced transparency (EIT) [19,20]. Numerous metamaterial configurations are reported in the literature particularly for sensing applications [21–24]. A special class of metamaterials is called hyperbolic metamaterials (HMMs) due to their hyperbolic dispersion relation. This specific type of dispersion arises from extreme anisotropy, one or two components of their permittivity/ permeability tensors being negative [25]. Several structures have been proposed to physically realize HMM, e.g., metal-dielectric multilayer structure [26], nanowire arrays [26], hyperlens [26] and multilayer fishnet [26]. Different material combinations render hyperbolic dispersion characteristics at different regions of the electromagnetic spectrum. One of the simplest ways to realize HMM is by arranging thin metal and dielectric layers, which are of subwavelength thickness, in sequential multi-layer structure. HMMs can also be realized using graphene-dielectric multi-layer instead of regular metal-dielectric multi-layer. A graphene-dielectric multi-layer structure can show hyperbolic dispersion property in Terahertz frequency region. This type of structures has been investigated both theoretically [27,28] and experimentally

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[29] in the literature. Conventional HMMs have found some applications, for example, in sub-wavelength imaging [30], extreme sensing [31] and wave-guiding [32,33].

A conventional metal-dielectric HMMs can support high- k volume plasmon polariton (VPP) or bulk plasmon polariton (BPP) modes due to their diverging optical density of states. These VPP modes arise due to the coupling between short-range (even) surface plasmon polaritons (SR-SPPs) in the individual metal-dielectric interfaces for metal-dielectric multilayer hyperbolic systems [34]. It has been experimentally demonstrated that using a sub-wavelength diffraction grating, these VPP modes can be excited in regular metal-based HMMs [31].

From theoretical perspective, graphene-based HMMs should also support VPP modes. Excitation of VPP modes in graphene-based HMMs is comparatively difficult due to large wave-vector mismatches between VPP modes and free-space wave. Using of Kretschmann configuration demands a material with very high refractive index, which is not physically possible yet. In this work, we propose a grating-integrated graphene-based HMM device for excitation of high- k VPP modes in the Terahertz frequency regime. A detailed theoretical and numerical studies of the excited VPP modes are carried out in this work. Feasibility of utilizing the proposed structural configuration as sensing and imaging platforms is also studied. It is found that the metallic grating induces 'Fano resonance' in the transmittance and reflectance spectra of the proposed graphene-based HMM and thus plays a vital role in exciting VPP modes, which can potentially be utilized in imaging and sensing applications for, e.g., chemical and biological analytes.

II. PROPOSED GRATING-COUPLED GRAPHENE HMM (GC-GHMM)

The proposed structure is illustrated in Fig. 1. The graphene HMM is composed of alternate layers of graphene and dielectric. The distance between any two consecutive graphene layers or the width of a dielectric layer is ' d '. The property of graphene-dielectric multilayer as hyperbolic metamaterial is explained in 'III. THEORETICAL ANALYSIS' section. A metallic grating is placed over the metamaterial with a period of ' a ', width of ' w ' and height ' h '. Light is incident from the top of the grating (along the negative z axis) when the device is numerically simulated using Finite-Difference Time-Domain (FDTD) technique. Grating coupling technique has been used to fulfill the required phase-matching condition. The metal grating can overcome the mismatch between the in-plane wave-vector of plasmon modes, β , and the incident wave, k_0 [35], according to equation (1).

$$\beta = k_0 \sin \theta \pm m \frac{2\pi}{a}. \quad (1)$$

here, θ indicates angle of incident, and ' m ' is a positive integer (1, 2, 3, ...).

The whole device is based on a silica (SiO_2) substrate, as shown in Fig. 1. Silica is chosen as the substrate material considering its favorable physical and optical properties for the proposed device. The most important requirement as a substrate for the growth of optical grade two-dimensional (2D)

Fig. 1: Proposed grating-coupled graphene-based hyperbolic metamaterial (HMM). A metallic grating with a period of ' a ', width of ' w ' and height of ' h ' is at the top of the HMM (the duty cycle of the grating is defined as, w/a). The HMM is shown composed of four alternate layers of graphene and the dielectric material. Thickness of each dielectric layer is ' d '. The whole device is based on a silica substrate.

or single-layer materials, like graphene, is its very low surface roughness (< 1 nm). It is reported in the literature that silica can be obtained to have a surface roughness as low as 0.5 nm and optical grade growth of graphene single layer on silica has already been demonstrated experimentally [36]. Also, there are some 2D substrate materials (e.g., hBN, WSe2 and MoS2) that can have surface roughness of this scale, but being 2D materials they are expensive and can be difficult to handle for the growth of another 2D material (graphene) on them. In terms of the optical transmission characteristics, silica glass can show good transmission efficiency of up to about $4 \mu\text{m}$ but it effectively acts as an opaque layer beyond that wavelength. Silica can still be used as substrate material for the device optimized to operate beyond this wavelength. In that case, reflectance spectroscopy, in lieu of transmittance spectroscopy, can be used to probe the VPP resonance in the device.

Regarding the practicality of the proposed structure, it can be said that a graphene- Al_2O_3 multilayer structure has already been practically realized and its hyperbolic dispersion characteristics are confirmed experimentally [29], as mentioned earlier. Chemical vapor deposition (CVD) technique was used for the growth of graphene layers on copper sheets and atomic layer deposition (ALD) technique for the growth of Al_2O_3 layers on graphene. The CVD-grown graphene layers were transferred onto the substrate and on the grown Al_2O_3 layers using poly-methyl methacrylate (PMMA) as the carrier material. In our proposed structural configuration, additionally we use a metal grating on top of the multilayered graphene- Al_2O_3 to aid in the excitation of high- k VPP modes. The thin metal film (e.g., silver film) for the grating can be deposited on the HMM using physical vapor deposition technique and then the deposited metal film can be patterned for the required grating parameters using state-of-the-art nanolithography and etching techniques.

III. THEORETICAL ANALYSIS

Strong interaction between photons and π -electrons of graphene can create charged oscillations known as graphene plasmons. Dispersion relation of graphene plasmons can be determined for TE and TM polarization as [37],

$$\text{TM mode : } \frac{i\sigma k}{\omega\epsilon_0\epsilon} + 2 = 0 \quad (2)$$

$$\text{TE mode : } \frac{i\sigma\omega\mu_0}{k} + 2 = 0 \quad (3)$$

where the symbols have their usual meanings. The in-plane wave-vector of graphene plasmons can be calculated as $\beta = \sqrt{\epsilon k_0^2 - k^2}$, k_0 is free-space wave-vector. For equations (2) and (3), a single layer graphene is considered to be surrounded by a dielectric with permittivity $\epsilon_0\epsilon$ and permeability μ_0 . Graphene conductivity can be calculated using expression in [38]. It is evident from equations (2) and (3) that the TM-polarized graphene plasmon modes have much larger wave-vectors than their TE counterparts. Larger wave-vectors result in higher confinement of plasmon modes. The better confinement of TM modes makes TM wave excitation suitable for plasmonic applications. So, we shall consider only the TM wave incidence on the device for theoretical and numerical analysis of VPP modes. With two graphene layers in close vicinity, coupling between two TM modes can cause TM dispersion in equation (2) to split into two modes: odd plasmon mode (long-range surface plasmon polaritons (LR-SPPs)) and even plasmon mode (short-range surface plasmon polaritons (SR-SPPs)). LR-SPP has a shorter wave-vector than its single layer mode and SR-SPPs has a longer wave-vector. It has been shown by Zhukovsky *et. al* [34] that in metal-dielectric multi-layer HMMs, these SR-SPP modes evolve into VPP modes, allowing the modes to propagate in transverse direction of the multi-layered structure. The dispersion relations for these two modes, LR-SPP and SR-SPP, for graphene plasmons can be shown to take the forms as follow:

$$\text{Odd mode : } \tanh(kd) = \frac{\sigma k}{i\omega\epsilon_0\epsilon} - 1 \quad (4)$$

$$\text{Even mode : } \tanh(kd) = \frac{1}{\frac{\sigma k}{i\omega\epsilon_0\epsilon} - 1} \quad (5)$$

here, ' d ' is the distance between two graphene layers or width of the dielectric layers. The equations of real and imaginary parts of $\beta (= \sqrt{\epsilon k_0^2 - k^2})$ for both of these modes indicate that the even mode has longer wave-vector than that of the odd mode.

Decreasing the distance ' d ' between the graphene layers causes splitting between odd and even modes to increase. From Fig. (2a) and equation (5), it is clear that any decrease in ' d ' causes SR-SPP modes to shift to lower frequency (or increasing wave-vector at a specific frequency). Furthermore, with increased coupling, increasing β makes it physically possible to evolve into high- k VPP modes in the graphene HMM.

Introducing three alternate layers of graphene-dielectric further splits each mode. The dispersion relation for such a three-way-coupled graphene Plasmon mode can be derived as:

$$\exp(-2kd) = \frac{\sigma k}{i\omega\epsilon_0\epsilon} \frac{\frac{\sigma k}{i\omega\epsilon_0\epsilon} \pm 4}{(\frac{\sigma k}{i\omega\epsilon_0\epsilon} - 2)^2} \quad (6)$$

Equation (6) is the dispersion relation for four modes, which can be written as:

$$\text{odd mode : } \tanh(ka) = \frac{2 - 2\frac{\sigma k}{i\omega\epsilon_0\epsilon}}{-\frac{\sigma^2 k^2}{\omega^2 \epsilon_0^2 \epsilon_r^2} + 2} \quad (7)$$

$$\text{even mode : } \tanh(ka) = \frac{2}{(\frac{\sigma k}{i\omega\epsilon_0\epsilon} - 2)^2} \quad (8)$$

Equation (7) and (8) each contains two modes: even mode in equation 7 contains SR-SPP1 and SR-SPP2 and odd mode in equation 8 contains LR-SPP1 and LR-SPP2. One of these three modes, SR-SPP1, shows further increase in wave-vector than SR-SPP mode. This mode is specifically illustrated in Fig. 2(b). As the number of graphene layers is increased, this mode shows gradual increase of wave-vector. This specific mode evolves to VPP mode for graphene-based HMM structure. All the modes mentioned above have higher in-plane wave-vector than the free-space wave-vector (SR-SPP1 mode has $\beta = 596 \text{ nm}^{-1}$ at 2 THz). A way to overcome this huge mismatch is to couple the incident wave to the HMM through grating. A superimposed plot of SR-SPP1 dispersion with equation (1) using several ' m ' values (using, $\theta=0$) is shown in Fig 2(c). Different values of ' m ' result in resonances at different frequencies. From the plot shown in inset, it is clear that $m = 3$ can excite SR-SPP1 mode at around 2 THz. But at higher frequencies (> 200 THz), the subsequent resonant frequencies get very close to each other (Fig. 2(c)).

Analytical calculation using more than three alternate graphene-dielectric layers is difficult. To understand the behavior of multilayered structure, FDTD method has been employed in this work. The behavior of graphene-based HMM can be approximated by considering infinite number of alternate graphene-dielectric layers using 'Transfer Matrix Method'. Transfer matrix for graphene can be written as,

$$G = \begin{bmatrix} 2 - \frac{\sigma k}{\omega\epsilon_0\epsilon} & \frac{\sigma k}{\omega\epsilon_0\epsilon} \\ -\frac{\sigma k}{\omega\epsilon_0\epsilon} & 2 + \frac{\sigma k}{\omega\epsilon_0\epsilon} \end{bmatrix} \quad (9)$$

$\epsilon_0\epsilon$ is the permittivity of the dielectric media surrounding the graphene layer and k is wave-vector in transverse direction. So the transfer matrix for a period of the HMM is $T = GD$, where D is the transfer matrix for the dielectric layer. We can determine the Bloch wave dispersion as, $\cos(\mathbf{Q}d) = (T_{11} + T_{22})/2$, where $\mathbf{Q}$ is Bloch wave-vector. The dispersion relation of Bloch wave is:

$$\cos(\mathbf{Q}d) = \cos(\mathbf{k}d) - \frac{i\sigma k}{\omega\epsilon_0\epsilon} \sin(\mathbf{k}d) \quad (10)$$

By expanding the *cosine* function up to $k^2 d^2/2$ and the *sine* function up to kd , we get the dispersion relationship for the graphene-dielectric multilayer as,

$$\frac{\mathbf{Q}^2}{\epsilon(\frac{1}{2} + \frac{i\sigma k}{\omega\epsilon_0\epsilon d})} + \frac{\beta^2}{\epsilon} = k_0^2 \quad (11)$$

Fig. 2: Coupled graphene plasmon, (a) real part of in-plane wave-vector for two layers of graphene with separation between the layers is 10, 25, 40 nm; (b) real part of SR-SPP mode for different number of graphene layers (2, 3); (c) using grating to excite plasmonic mode for three layers configuration. ‘ m ’ is from equation (1). Inset shows the results for the lower value of ‘ m ’ ($m = 1, 2, 3, 5$).

Hyperbolic dispersion appears when,

$$Im(\sigma) > \frac{\omega \epsilon_0 \epsilon d}{2} \quad (12)$$

For dielectric with $\epsilon = 2.5$, hyperbolic dispersion appears for frequency $< f_c = 121$ THz ($\lambda > 2.5\mu m$). Increasing dielectric constant of the dielectric material causes the cut-off frequency (f_c) to decrease, and vice versa. In the hyperbolic dispersion regime, a larger value of β does not result in an imaginary value of $\mathbf{Q}$, transverse wave-vector (equation 11). VPP mode can propagate in transverse direction inside HMM. In material with elliptical dispersion, this transverse propagation is not possible, as higher β value causes the wave to become evanescent (due to imaginary $\mathbf{Q}$) in the transverse direction.

IV. NUMERICAL ANALYSIS

A. Methodology

An FDTD method has been employed to solve the Maxwell’s equations numerically for the geometry shown in Fig 1. The structure, being semi-infinite along the y direction, is simulated in the x - z plane. Perfectly matched layer (PML) boundary condition is employed along the z boundaries of the FDTD domain and periodic boundary condition along its x boundaries. In the simulation, graphene was modeled as a 2D rectangle with zero thickness. As a 2D material, graphene is modeled to support only surface current, J_s , in optical engineering. In our numerical simulation, this is implemented by using the corresponding Maxwell’s equation as, $\nabla \times \mathbf{H} = \mathbf{J}_s = \sigma \mathbf{E}$. For graphene at $z = 0$, the magnetic field surrounding the graphene layer is calculated as, $H(z \rightarrow 0^+) - H(z \rightarrow 0^-) = \sigma E(z = 0)$. A non-uniform meshing scheme with finer meshes in the vicinity of graphene layers and metal grating region has been used to maintain good accuracy of computation. Light is incident on the device from the top (along the negative z axis) as shown in Fig 1. Simulation is carried out only for TM-polarized incident electromagnetic wave, the explanation for which is provided earlier in the section ‘III. THEORETICAL ANALYSIS’. Conductivity of graphene has been computed

from ref. [38]. Unless otherwise specified, Fermi energy and scattering rate of graphene are realistically assumed to be constant at 0.64 eV and 0.196 meV, respectively. Simulation was performed for a broad range of frequencies spanning from 2 THz to 80 THz, since the structure remains in hyperbolic dispersion regime in this whole range.

B. Results

Reflectance and transmittance spectra of the proposed GC-GHMM is shown in Fig. 3. These results are obtained for an HMM with six alternate layers of graphene and Al_2O_3 , which shows hyperbolic dispersion property for $f < 70$ THz with the graphene layers having a chemical potential $\mu = 0.64$ eV. Several peaks are found in the transmittance spectrum corresponding to plasmonic VPP modes (confirmation is made later in this sub-section). Transmittance is measured along the transverse direction of the HMM. High transmittance in the low frequency range indicates the propagating VPP modes. SR-SPPs normally cannot propagate along the transverse direction due its large imaginary value of transverse wave-vector. However, inside HMM, the SR-SPP modes evolve into VPP modes with higher in-plane wave-vectors which can propagate in transverse direction because of its real transverse wave-vector $\mathbf{Q}$. Fig. 3 shows the results for the case with the graphene layers having a chemical potential, $\mu = 0.64$ eV, and $\hbar\gamma = 0.196$ meV, and with the silver grating having a period of 800 nm and a duty cycle of 0.5 (Duty cycle of a grating is defined as the ratio of its width (w) to its period (a), w/a). As we move toward higher frequencies, the resonant modes start to get closer to each other, which is clear from Fig. 2(c). The graphene layers with a chemical potential $\mu = 0.64$ eV make the HMM fully transparent at $\omega > 2(\mu/\hbar) \approx 309$ THz. However, a 97% transmission at 60 THz marks the excitation of VPP modes inside HMM at that frequency.

The rise and fall around the transmission peak, especially in the lower frequency regime of the transmission spectrum (Fig 3(c)), is found to be asymmetric in nature. This sort of asymmetry in the resonance spectrum can be attributed to Fano resonance, which is due to the interaction between two plasmon modes with different amount of losses, the metallic

Fig. 3: Broadband reflectance and transmittance spectra, (a) from 40 to 80 THz; (b) from 12.5 to 20 THz; and (c) from 2.5 to 7 THz. Here, the GC-GHMM had 6 alternate layers of graphene and Al_2O_3 with each Al_2O_3 layer has a thickness of 10 nm. The inset of (a) shows a closer look between 59 to 66 THz with three modes.

grating plasmon and graphene plasmon modes. As discussed by Chen *et al.* [39], metal plasmon is a high ohmic loss plasmonic mode and provides a broad spectrum while low-loss graphene plasmon gives a discrete spectrum, resulting in Fano resonance. It is to be noted here that the angle of incidence of electromagnetic wave has no influence on this asymmetry, as confirmed by the simulation. From the figures shown in Fig. 2, the resonance frequencies can be found as 3.87, 4.89, 5.83, 16.45, 52, 60.7 and 65.2 THz with the Q-factors of 29, 30, 32, 1, 200, 260 and 300, respectively. There are several resonances beyond these points. To confirm the formation of VPP modes, the electric-field (E-field) patterns are analyzed at these resonance frequency points using the same numerical technique. The E-field patterns induced in the proposed structure at those frequency points are illustrated in Fig. 4.

Before the E-field patterns of Fig. 4 are examined, a basic description about the origin of VPP modes is necessary. The physical origin of the excitation of the VPP modes in a hyperbolic metamaterial is complex as explained analytically in ‘III. THEORETICAL ANALYSIS’ section of the paper. The physical origin of VPPs starting with its basics can qualitatively be summarized as follows. VPPs are a type of plasmons that are excited in a material bulk due to interactions among multiple surface plasmon modes from nearby surfaces. We know that the initial surface plasmon polaritons are excited due to resonance energy transfer from photons of compatible wave-vector to the oscillations of surface electrons of a material (metal/semiconductor). In our case, the resonances occur with the surface electrons of graphene at the graphene- Al_2O_3 interfaces, which initially excites surface plasmon polariton (SPP) modes. Subsequent interactions among SPP modes of adjacent interfaces may excite the plasmons in the bulk of the metamaterial. These bulk plasmons are termed as VPPs and their E-field profile normally has a characteristic shape of ‘V’ angle. An important condition of resonance requires that the in-plane wave-vector of the incident photon be much greater than the free-space wave-vector, which is determined by the dispersion relation of the plasmons in the metamaterial. In our case, this condition is achieved by using metal grating at the very top of the metamaterial. It affects the wave-vector

of the transmitted waves as per grating equation (1). So, the resonance frequencies are determined by the intersections of the grating equation (1) with the dispersion curve of the graphene HMM, and they are shown in Fig. 2(c). To ensure that each of these resonances is actually caused by the excitation of VPPs, the electric field profiles in the bulk of the metamaterial are needed to be examined at those frequencies. Transverse propagation of wave and characteristic ‘V’ angle of the electric field profile confirm that the plasmons excited at that frequency are due to VPP modes.

Propagation of the VPP modes along transverse direction is clear from Fig. 4. Appearance of characteristic ‘V’ angle is a signature of the excited VPP modes [40]. This characteristic angle becomes more obvious in higher frequency regime (e.g., Figs. 4(a), 4(b) and 4(c). In high frequency regime, plasmonic interference pattern appears due to interference between the two high- k modes of adjacent graphene layers. As the operating wavelength increases (frequency decreases), graphene plasmon modes become less confined to a single layer. This can be explained with reference to Fig. 2 as follows: As wavelength increases, β/k_0 tends to reduce toward 1, and a lower β signifies less confinement of electromagnetic wave. Clearly from Fig. 4(a) to 4(g), progressive increase in plasmon period, except in Fig. 4(d), confirms that claim. The E-field pattern of Fig. 4(d) confirms that there are no VPP modes excited in the structure for the frequency of 16.45 THz. This can be explained with reference to Fig. 3(b) that shows a symmetric linewidth around the resonance peak of the transmission spectrum at 16.45 THz, which suggests the existence of only one type of plasmon modes for this resonance, and hence the absence of Fano resonance. As can be seen from the E-field distribution in Fig. 4(d) that there are only metallic grating plasmon modes and no graphene plasmon modes excited at this frequency. So no VPP modes are induced at this frequency, since, as stated earlier, coupling between at least two types of plasmon modes are necessary for excitation of VPP modes.

It is obvious from Fig. 2 that the high-frequency plasmonic modes also have high in-plane wave-vectors. This existence of high in-plane wave-vector with low graphene plasmon period shows potential for the proposed structure as an imaging platform. The resonances shown in Fig. 4 experience different

Fig. 4: Induced electric-field patterns at, (a) 65.2 THz, (b) 60.7 THz, (c) 52 THz, (d) 16.45 THz, (e) 5.36 THz, (f) 4.89 THz, and (g) 3.57 THz. Here, light is incident from the top.

levels of field enhancement and field confinement, as shown in Table I. Field enhancement measures the maximum intensity of the induced E-field at a particular resonant frequency. Field confinement measures the ratio of the effective wavelength of the excited graphene plasmons to the resonant wavelength. Effective plasmonic wavelength is measured as the spatial distance between two consecutive peak positions in the interference pattern. No graphene plasmon modes are induced at 16.45 THz, as explained earlier. Field confinement is higher at lower frequencies. However this will be a misleading result to use this device as imaging platform in that lower frequency range. In order to achieve high resolution imaging platform, effective wavelength should be as low as possible, which is only possible at higher frequencies for GC-GHMM. At a lower frequency, the period of graphene plasmon increases, causing the resolution to worsen. However, beyond a certain range, graphene plasmon loses its high- k characteristics (Fig. 2(a)) and the wavelength gets larger. It is optimal to use GC-GHMM as imaging platform in 4-8 μm range.

The resonance mode of GC-GHMM is extremely tunable. Several parameters have been changed to investigate the

TABLE I: Plasmonic field confinement and field enhancement at different frequencies

Resonance frequency (THz)	Field enhancement	Effective wavelength of Graphene Plasmon (nm)	Field confinement
65.2	18	100	46
60.7	16	96	51
52	16	104	62
16.45	3	-	-
5.36	30	385	145
4.89	16	345	175
3.57	22	380	221

tunable behavior of the GC-GHMM: dielectric material and its thickness, total number of alternate graphene-dielectric period/layers, chemical potential and scattering rate of graphene layer, period and duty cycle of grating. Effects of all these parameters have been analyzed using numerical FDTD method. Reflectance spectrum from 2.5 to 7 THz has been shown in Fig. 5 for all these cases.

Increasing dielectric permittivity causes the HMM region to red shift (equation (12)). Same trend can be found from

Fig. 5: Reflectance spectra of the proposed structure as a function of

(a) dielectric layer materials, (b) dielectric layer thickness, (c) number of graphene-dielectric periods, (d) chemical potential of graphene, (e) grating period, and (f) grating duty cycle.

Fig. 6: Plasmonic interference pattern for (a) graphene-10 nm SiO_2 HMM at 65.57 THz, (b) graphene-10 nm Al_2O_3 with Ag grating of 1200 nm period at 57.6 THz, (c) graphene-20 nm Al_2O_3 at 60.5 THz, (d) graphene-10 nm Al_2O_3 with 0.1 grating duty cycle at 64.5 THz, (e) four alternate layers of graphene-10 nm Al_2O_3 at 64.6 THz, and (f) graphene-10 nm Al_2O_3 with Ag grating of 1200 nm period at 65.13 THz.

equations (2), (5) and (8). From Fig. 5(a), it is clear that same red shift has occurred in the numerical simulation using the dielectric material with increasing dielectric constant (SiO_2 , Al_2O_3 , Si_3N_4 in that order). With increasing thick-

ness of dielectric layer, coupling between graphene layer is weakening causing the graphene plasmon mode to shift to higher frequency. Furthermore, increasing distance between graphene layers causes some high order plasmonic modes to

disappear (Fig 2(a)). Blueshift of resonances with increasing dielectric thickness is obvious from Fig. 5(b). Increasing the number of graphene-dielectric layers can make the dispersion of the HMM material an ideal hyperbolic dispersion [24]. This idea has also been clear in Fig. 2(b). Clear redshift as seen in Fig. 5(c) supports that. Changing chemical potential of graphene causes graphene optical conductivity to change. Increasing chemical potential causes the inter-band transition to occur at higher frequency, resulting in an overall blueshift for the resonant mode. Effect of grating period is explained in equation (1). Changing period can cause several new modes to appear as excitation with new wavevector is possible. Some of these is visible in Fig. 5(e). Changing the duty cycle does not affect the positions of the resonant modes too much. But decreasing it to a very low value can cause the perturbation of incident wave-front insignificant to excite plasmonic modes in graphene. Changing substrate material does not show any significant changes to the plasmonic spectra of the device. The tunability of the graphene VPP modes is a good criterion for GC-GHMM to be used in tunable sensor design. A slight change in dielectric constant can cause the VPP resonance modes to shift in frequencies and this can be exploited as a sensor enabling physics.

In view of the device realization, the most critical design parameter to control would presumably be the chemical potential of the graphene layers. Changing chemical potential for graphene requires an external electrical gating circuit with the requirement of electrical interface to each graphene layers in the device [29], which may make it very critical to be implemented and optimized. The structural design parameters of the proposed device (dielectric layer material, dielectric layer thickness, number of graphene-dielectric layer periods, metal grating period and metal grating duty cycle) can well be optimized and fabricated within the errors determined by the process tolerances of the state-of-the-art material growth and nanofabrication technologies.

C. GC-GHMM as Imaging Platform

As hinted earlier, GC-GHMM can be used as an imaging platform in the wavelength range of 4-8 μm . To find out the optimal condition of GC-GHMM as an imaging device, all the parameters mentioned above has been tried and interference pattern along with field enhancement have been calculated. Several electric field profiles have been shown in Fig. 6. Two best cases (smallest spatial imaging resolution) are shown in Fig. 7 with the corresponding plasmonic interference patterns shown enlarged at their insets. It is to be noted here that the 'imaging resolution' of an imaging device indicates the minimum distance by which two objects must be spatially separated to be identified separately by the device. It is calculated as the half of the spatial distance between two same-phase points of the induced electric field pattern or half of the spatial distance at which the plasmonic interference pattern repeats itself..

For an Ag grating with a period of 800 nm and a duty cycle of 0.5, plasmonic interference pattern repeats itself at a spatial distance of 35 nm for GHMM with 10 nm SiO_2 at an

incident wavelength of 4.57 μm (65.57 THz) (Fig. 6(a) and Fig. 7(a)). Here, a six times enhancement of field intensity and 130-fold increase in the field confinement have been achieved, which is way beyond the diffraction limit with an imaging resolution (spatial) of 17.5 nm. With increasing dielectric layer thickness, interaction between graphene plasmons of adjacent layers diminishes and interference pattern eventually vanishes (Fig. 6(c)). For an Ag grating with a period of 1200 nm and a duty cycle of 0.5, plasmonic interference pattern repeats itself at a spatial distance of 30 nm at 4.6 μm wavelength excitation, which results in 153-fold increase in the field confinement (Fig. 6(f) and Fig. 7(b)) and an imaging resolution (spatial) of 15 nm. Interference pattern actually changes with grating property (period and duty cycle) and also with the HMM parameters. All these findings make our proposed GC-GHMM potentially a strong candidate for infrared imaging platform.

D. GC-GHMM as sensing Platform

We can utilize the spectral change of resonance mode with refractive index to use GC-GHMM as a sensor. For proof of concept, a graphene- Al_2O_3 HMM with 6 alternate periods of graphene-10 nm Al_2O_3 has been studied for its performance as a sensing device where the third Al_2O_3 layer is used as the sensor platform, i.e this layer has been replaced with sensing layer. FDTD method has been used to numerically solve the Maxwell's equations for this structure for three different refractive indices of the sensing layer; 1.3, 1.4 and 1.5. Results of the simulation are shown in Table II. The VPP modes at low frequencies show relatively higher sensitivities to the change in refractive index of the sensing layer compared to the modes at higher frequencies. The spectral shift is also depicted in Fig. 8.

As can be seen from Table II, a very high sensitivity of 11,050 nm/RIU can be achieved from this sensor configuration for sensing materials having refractive indices around 1.5 when operated at the lower THz regime of the spectrum. Although most chemical and biological solutions have refractive indices in the range of 1.32 - 1.38 [41], there are some biomolecular proteins that are reported to have refractive indices as high as 1.6 [42]. Moreover, at the lower THz regime of the spectrum, the sensitivities of the device are also very high (can be close to 10,000) for the refractive index range of 1.34 - 1.4, which is expected to cover its applications to many chemical and biological samples.

We have studied the excitation of the VPP modes in the proposed structure over a broad range of terahertz frequencies ranging from 2 THz – 80 THz. However, the operating frequency band for a specific sensing application will definitely be a small sub-band(s) of the whole VPP excitation spectrum. The sensor operating band may roughly be estimated from the results provided in Table II to be around 3 – 5 THz (based on sensitivity only). The operating band can be in a different region of the original VPP spectrum (2 –80 THz) depending on the constraints of the specific applications and optimization criteria. A more optimized operating band or multiple sub-bands of a sensing device can be determined by multi-parameter optimization of the sensor device for the

Fig. 7: Plasmonic interference patterns of GC-GHMM. (a) with a silver grating having a period of 800 nm and a duty-cycle of 0.5 on graphene-10 nm SiO_2 HMM. (b) with a silver grating having a period of 1200 nm and a duty-cycle of 0.5 on graphene-10 nm Al_2O_3 HMM. The insets in both figures show two enlarged interference peaks. Distance between the two peaks is also shown.

particular constraints of the applications, which we expect to study in a future work.

Fig. 8: Reflectance spectra of GC-GHMM for three different refractive indices of the sensing layer

TABLE II: Sensitivity of different VPP modes.

Refractive index (RI) of the sensing layer	Resonance position (nm)	Sensitivity (nm/RIU)
1.3	4542	-
1.4	4573	310
1.5	4605	320
1.3	4922	-
1.4	4959	370
1.5	4984	250
1.3	5694	-
1.4	5760	370
1.5	5794	250
1.3	55419	-
1.335	74572	2338
1.34	74655	9764
1.4	75244	10517
1.55	76901	11050
1.62	77607	10588

V. CONCLUSION

In this report, we propose a graphene-based HMM structure with integrated metal grating for efficient coupling of the electromagnetic wave to the structure to facilitate efficient excitation of high- k VPPs. The semi-analytical expression of dispersion relation for the proposed structure is formulated and has been found to be indicative of the origins of these sort of modes in the structure. To validate the analytical results, numerical simulation has been performed and field confinement and field enhancement of the VPP modes have been determined. Plasmonic interference pattern is observed in the nano-cavity formed between adjacent graphene layers. This enhanced plasmonic interference phenomena of the proposed structure can potentially be used as imaging and sensor platforms in the infra-red frequency regime. Furthermore, it has been shown that the periodic pattern of the plasmonic interference and the spectral positions of the VPP modes can be tuned in several ways and thus the proposed grating-integrated graphene-based HMM provides additional degrees of freedom in designing appropriate resonance wavelength for the desired applications. However, the design optimization of the proposed sensor configuration for a particular application with specified constraints, and evaluation of its robustness against variations in the design parameters are not carried out in this work and can be studied in future.

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