Strong interaction between graphene and localized hot spots in all-dielectric metasurfaces

Shuyuan Xiao¹, Tingting Liu¹, Chaobiao Zhou³, Xiaoyun Jiang¹, Le Cheng³, Yuebo Liu⁴ and Zhong Li⁵,6

1 Institute for Advanced Study, Nanchang University, Nanchang 330031, People’s Republic of China
2 Laboratory of Millimeter Wave and Terahertz Technology, School of Physics and Electronics Information, Hubei University of Education, Wuhan 430205, People’s Republic of China
3 Wuhan National Laboratory for Optoelectronics, Huazhong University of Science and Technology, Wuhan 430074, People’s Republic of China
4 School of Electronics and Information Technology, Sun Yat-sen University, Guangzhou 510006, People’s Republic of China
5 Center for Materials for Information Technology, The University of Alabama, Tuscaloosa, AL 35487, United States of America
6 Department of Physics and Astronomy, The University of Alabama, Tuscaloosa, AL 35487, United States of America

E-mail: syxiao@ncu.edu.cn

Received 26 March 2019, revised 3 June 2019
Accepted for publication 11 June 2019
Published 15 July 2019

Abstract
The active photonics based on the two-dimensional material graphene have attracted a great deal of interest for developing tunable and compact optical devices with high efficiency. Here, we integrate graphene into the Fano-resonant all-dielectric metasurfaces consisting of silicon split resonators, and systematically investigate the strong interaction between graphene and the highly localized hot spots inside feed gaps in the near infrared regime. The numerical results show that the integrated graphene can substantially reduce the Fano resonance due to the coupling effect between the intrinsic absorption of graphene with enhanced electric field in the localized hotspot. With the manipulation of the surface conductivity via varying Fermi level and the layer number of graphene, the Fano resonance strength obtains a significant modulation and is even switched off. This work provides a great degree of freedom to tailor light-matter interaction at the nanoscale and opens up avenues for actively tunable and integrated nanophotonic device applications, such as optical biosensing, slow light and enhanced nonlinear effects.

Keywords: graphene, dielectric metasurfaces, Fano resonance, optical modulation

Supplementary material for this article is available online

(Some figures may appear in colour only in the online journal)

1. Introduction
The confinement of electromagnetic radiation within nanometresized scale associated with of strong localized electromagnetic field enhancement is one of the most important and fundamental strategies in light-matter interaction engineering [1]. The ability of plasmonic metasurfaces to break the diffraction limit and concentrate the light into subwavelength volumes provides unprecedented opportunities to convert optical radiation into intense, localized field distributions. The typical approach to generate and control the localized field enhancement is the excitation of Fano resonances, as
suggested in a variety of plasmonic metasurfaces composed of the planar arranged nanostructured metal building blocks [2–7]. However, high intrinsic losses and irreversible photothermal conversion process of traditional metal resonators have always been a challenge limiting the quality-factor (Q-factor) in practical optical devices. As an alternative to metal, high-index low-loss dielectric materials, such as silicon, germanium and tellurium, have recently risen to prominence in the nanophotonics toolkit [8, 9]. The Mie resonance behavior of dielectric enables the realization of low-loss functional devices with high efficiency and exotic functionalities. Similar with the plasmonic resonance in metal metasurfaces, all-dielectric metasurfaces support strong Fano resonance and electromagnetic field enhancement in the optical and near-infrared spectral range [10–14]. Unlike metal metasurfaces with concentrated electromagnetic fields in the surrounding medium, the fields in dielectric metasurfaces are confined within the resonators, severely hindering the practical applications. Solutions have been suggested to introduce the feed gaps in the dielectric resonant nanostructures, which would confine a larger portion of electromagnetic energy into nanoscale hot spots within the gap [15–19]. The feed-gapped dielectric metasurfaces serve as an ideal platform for further enhancing the interaction between light and the surrounding medium, making them promising candidates for highly sensitive optical biosensors, slow light, high-order harmonics generation, surface-enhanced enhanced Raman scattering and luminescence enhancement of quantum dots.

Recently, a new popular tendency in the research field of metasurfaces is the realization of actively controllable resonance responses, which would add more degrees of freedom in tailoring light for the development of tunable, reconfigurable and ultracompact optical devices [20]. On this issue, a vast number of tuning and switching schemes have been demonstrated in plasmonic structures of metal metasurfaces, including the mechanical reconfiguration [21, 22], and the combination with phase-change materials or photosensitive materials [23–26]. Subsequently, some of these modulation strategies have been extended to dielectric metasurfaces, for instance, the combination of all-dielectric metasurfaces with optomechanical system [27], the temperature dependent refractive-index change of amorphous liquid crystal or silicon material [28–31]. Nevertheless, the modulation time constants of these strategies are typically on the order of 10 μs to 1 ms, setting an obstacle for the real-time modulation. Very recently, a newly emerging two-dimensional (2D) material, graphene, has attracted considerable attention for dynamically controlling resonance response of metasurfaces, since the surface conductivity of graphene is actively tunable via shifting the Fermi level under an external bias voltage within a wide regime [32–34]. Moreover, the relaxation time of the excited carriers in graphene is on the order of picosecond [35, 36]. These exceptional properties makes graphene a better competitor than other active materials to be combined with metasurfaces for ultrafast control of optical resonances [37–43]. In this respect, researchers have been inspired to incorporate graphene with all-dielectric metasurfaces for active tunability. For instance, the combination of dielectric metasurfaces with graphene layer is proposed to achieve tunable transmission of the trapped modes for optical modulator [44, 45]. However, in these pioneering works, the field enhancements are confined inside the dielectric resonators, which limits the interaction with graphene and degrades the efficiency of the functional devices to an extent.

In this work, we provide a systematic investigation on the interaction between graphene with the localized hot spots based on feed-gapped all-dielectric metasurfaces in the near infrared regime. The unique feature of the metasurfaces, consisting of a pair of asymmetric split silicon bars is that the dielectric resonators support extremely high Q-factor Fano resonance and generate strong localized hot spots within the gaps. With graphene covered over the metasurfaces, the Fano resonance strength exhibits a remarkable modulation due to the strong interaction of the enhanced electric field with graphene. The interaction effect is investigated in great detail by changing the gap width, manipulating the surface conductivity via varying Fermi level and the layer number of graphene. To the best of our knowledge, this is the first investigation of the interaction between graphene and localized hot spots of Fano resonance in all-dielectric metasurfaces, offering great prospects for designing actively tunable and integrated nanophotonic devices with intriguing functionalities.

2. The geometric structure and numerical model

The schematic of the designed hybrid graphene-dielectric metasurfaces is illustrated in figure 1(a). The unit cell of the all-dielectric metasurfaces is shown in figure 1(b), following the classic design of feed-gapped structure to generate the hot spots, which consists of two silicon split nanobar resonators periodically patterned on a silica substrate [17, 18]. The periods along the x and y directions are the same as 900nm. The two asymmetric parallel silicon nanobars have slightly different lengths of 700nm and 750nm, and share the same width of 200nm, as well as the same thickness of 160nm. The feed gaps are introduced here and each of the two silicon nanobars has a 25nm wide groove in the center for the enhancement of the interaction between the fields and the surrounding medium. The graphene layer is then covered over the dielectric silicon nanobars in a continuous pattern. The dielectric particles with different geometries have been widely employed as building blocks of the metasurface due to their low intrinsic loss and especially their easy fabrication using top-down method. The graphene layer grown from the chemical vapor deposition can be transferred to the dielectric metasurfaces using standard transfer techniques [46].

Numerical simulations of the hybrid metasurfaces are carried out using the finite-difference time-domain (FDTD) method. In the calculations, the periodical boundary conditions are used in the x and y directions, and the perfectly matched layer is employed in the z direction. The plane waves are incident along −z direction and provide an electric field polarized along the x direction. The silicon and the silica are assumed to be lossless with the constant refractive index of $n_{Si} = 3.5$ and $n_{SiO_2} = 1.4$ [47]. The graphene
over the all-dielectric metasurfaces can be modeled as a 2D sheet and the surface conductivity is governed by the random phase approximation (RPA) in the local limit. The conductivity of graphene is related to the Fermi level $E_F$ and includes the interband and intraband contributions as follows [48, 49],

$$
\sigma_g = \sigma_{\text{intra}} + \sigma_{\text{inter}} = \frac{2e^2 k_B T}{\pi \hbar^2} \left( \frac{i}{\omega + i\tau} - \frac{1}{\ln \left( \frac{2 \cosh \left( \frac{E_F}{2k_B T} \right) \right)} \right)
$$

(1)

where $e$ is the electron charge, $k_B$ is the Boltzmann constant, $T$ is the environment temperature with a constant value of 300 K here, $\hbar$ is the reduced Planck’s constant, $\omega$ is the incident light frequency, and $\tau$ is the carrier relaxation time. $\tau$ is calculated from $\tau = (\mu E_F)/(e v_F^2)$ and depends on the carrier mobility $\mu$, the Fermi level $E_F$ and the Fermi velocity $v_F$. In accordance with the experimental results in [50], we set $\mu = 10000 \text{ cm}^2 \text{ V} \cdot \text{s}^{-1}$ and $v_F = 1 \times 10^6 \text{ m s}^{-1}$ in calculating the conductivity of the doped graphene. Therefore, the optical conductivity of the graphene can obtain a continuous manipulation ($0 \sim e^2/4\hbar$) by changing the Fermi level, as depicted in figure 2. The figures 2(a) and (b) plot respective variation of the real part and imaginary part of the graphene conductivity as incident light frequency and Fermi level increases. Because the interband contribution to graphene conductivity will be blocked once the Fermi level exceeds the Dirac point by half of the photon energy ($E_F > \hbar \omega/2$), the real part of the conductivity will rapidly reduce to around zero when the Fermi level is larger than the critical value. Hence, a clear boundary line can be observed in figure 2(a). On the contrary, the imaginary part of graphene conductivity in figure 2(b) shows a continuous increase due to the significant contributions of the intraband transition as the Fermi level increases across the critical value. The unique property of the graphene conductivity enables the flexible tunability of the localized hot spots in the near infrared regime.
3. Simulation results and discussions

To begin with, the transmission spectra of the all-dielectric metasurfaces composed of silicon split nanobars are presented in figure 3(a). Without the presence of the graphene layer, one can clearly observe a sharp asymmetric Fano dip at 213.36 THz in the regime of interest. Due to the reduced intrinsic losses of silicon material, the Fano resonance of the structure exhibits a high $Q$-factor. The $Q$-factor in a typical Fano resonance can be obtained through fitting the Fano line shape by the following formula [51],

$$T = |a_1 + ia_2 + \frac{b}{\omega - \omega_0 + i\gamma}|^2,$$

where $a_1$, $a_2$ and $b$ are in general real constants for fitting, $\omega_0$ is the central resonance frequency and $\gamma$ is the damping rate of the resonance. The $Q$-factor is then estimated from $Q = \omega_0/(2\gamma)$ as 1215.48.

The distribution of the corresponding electric field $E/E_0$ at the dip of the transmission spectrum is presented in figure 3(b), where $E$ and $E_0$ are the amplitudes of the local electric field and the incident electric field, respectively. The Fano resonance results from the anti-phased oscillation of displacement currents of the two split nanobar resonators with accumulated polarization charges. In particular, a large amount of opposite charges has been confined at the two sides of the gaps, leading to a large portion of electromagnetic energy density localized at the gap and, finally, a significant field enhancement within the gaps. The introduction of the feed gaps at the center of the silicon nanobars enables the further enhancement of the localized hot spots inside the gaps. Consequently, the high $Q$-factor and the strong localized hotspots in the designed all-dielectric metasurface allows the enhancement of the interactions between the light and the surrounding medium.

Next, the Fano resonance characteristics of the structure are investigated for the two cases with and without the graphene layer on different feed-gapped nanobar arrays, as shown in figures 4(a)–(d). Without the presence of the graphene layer, the asymmetric Fano shapes can be observed in transmission spectra for different gapped nanobar arrays. The variations of the feed gap widths in silicon nanobars of the metasurface provide the freedom to engineer the asymmetry degrees of the unit cell in the y direction, giving rise to the modulation of the high $Q$-factor resonances with significant localized hot spots inside the gaps. As the gap width of the silicon nanobars increases from 25 to 150 nm, the resonance frequency shows a blue shift since the increase of feed gap width leads to the reduction of the effective length of the silicon nanobars. The $Q$-factor of the resonances gradually decreases from 1215.48, 1128.07, 1052.06 to 985.19 as the gap width increases from 25, 50, 100 to 150 nm, arising from the increasing radiative losses. In addition, the electric field distributions of the different gapped dielectric metasurfaces are plotted in figures 5(a)–(d). As the gap of the silicon nanobars becomes wider, the electric fields concentrated at ends of the resonators become gradually weaker and the accumulation of the opposite charges at the two sides of the gaps shows a declining tendency. The decreasing proportion of the electromagnetic energy results in the smaller localized hot-spot amplitude.

With the presence of graphene covered over the dielectric metasurfaces, although the trend of the blue shift in the resonance frequency is exactly retained, the resonance strength of Fano resonance undergoes a remarkable modulation, which indicates a strong interaction between graphene and the localized hot spots. As shown in figures 4(a)–(d), the transmission amplitude of the resonance rapidly decreases when the undoped graphene layer with a fixed Fermi level $E_F = 0$ eV (the optical conductivity of $e^2/\hbar$) is placed on the silicon nanobar arrays. To characterize the amplitude modulation in a quantitative way, we introduce the absolute value of modulation depth as $\Delta T = |T_g - T_0| \times 100\%$, where $T_g$ and $T_0$ are the transmission coefficients at the resonance dip for the dielectric metasurfaces with and without graphene, respectively. The modulation depth can be calculated as $\Delta T = 55.08\%, 58.96\%, 63.32\%, 62.12\%$, and the $Q$-factor of the resonances accordingly decreases from 131.07, 129.14, 121.25 to 115.07 for the gap width of 25, 50, 100, 150 nm, respectively.
Figure 4. The simulated transmission spectra of the dielectric metasurfaces with and without the graphene layer in silicon nanobar arrays with different gap widths.

Figure 5. The distributions of the electric field $E/E_0$ at the resonance frequency for silicon nanobar arrays with different gap widths (a)–(d) without the graphene layer and (e)–(h) with the presence of the graphene layer.
To understand the interaction mechanism, the corresponding electric field distributions at the Fano resonances with the graphene layer are compared in figures 5(e)–(h) to reveal the coupling effect between graphene layer and the localized hot spots. As mentioned previously, the high $Q$-factor and the strong localized hot spots provide a platform for the enhanced interaction between light and the surrounding medium. As the only lossy material in the hybrid structure, the monolayer graphene strongly couples to the incident light with its intrinsic absorption once it is integrated into the all-dielectric metasurfaces. According to equation (1), the interband contribution is dominant in the conductivity at near infrared frequencies, and the high conductivity of graphene leads to a remarkable light absorption. As a result, the electric field within the feed gaps dramatically decreases, leading to the shrunken outline of the localized hot spots and the reduction in Fano resonance strength, which corresponds to the significant change in the transmission coefficients. By contrast, we also present the modulation of the undoped graphene on the strength of Fano resonance in the dielectric metasurfaces consisting of the continuous nanobars without feed gaps (see supplementary material figure S1 (stacks.iop.org/JPhysD/52/385102/mmedia)). The modulation depth of only 48%, is lower than that of the feed-gapped structure due to the severely limited interaction between graphene and the electric field inside the continuous dielectric nanobars.

In figure 6, the dependences of the maximum field enhancement in the feed gaps and the modulation depth upon the feed gap width are summarized for the designed metasurfaces. The maximum field enhancement factor gradually decreases from 120 to 57, with an increasing gap width from 25 to 150 nm, because the coupling effect between the two parts of the split bar becomes weaker, and the accumulation of the opposite charges at the two sides of the gap gradually reduces with larger gap width. The modulation depth $\Delta T$ of the transmission strength increases from 55% to 63% during the increase in the gap width from 25 nm to 100 nm, and reaches the maximum at 64% for the gap width of 125 nm, implying even stronger interaction between graphene and the localized hot spots. The opposite tendency can be attributed to the fact that the volume for the interaction becomes larger with larger gap width and a larger proportion of electromagnetic field in the gap would interact with graphene. However, the modulation depth $\Delta T$ does not keep increasing if the gap width is more than 125 nm. The modulation depth $\Delta T$ decreases to 62% for the gap width of 150 nm, since the proportion of the electromagnetic field in the gap would not continue to increase resulting from the counteraction between the weaker field enhancement and the larger gap width for such large gap width. Hence, the field enhancement of the dielectric structure can be further increased with a shorter gap, which exactly satisfies the requirements of some applications including nonlinear optics and enhanced Raman scattering, in some other specific applications such as optical modulation as well as biosensing, the optimum width of the feed gap needs to be carefully traded off (in the present situation $g = 125$ nm) with the modulation depth limit for reconfigurable and compact devices.

Next we investigate the modulation potential of monolayer graphene arising from the continuously tunable conductivity via shifting the Fermi level. In the hybrid metasurfaces here, the feed gap of the silicon nanobars is fixed as 25 nm in width, and the Fermi level of graphene is varied as $E_F = 0$ eV, 0.5 eV and 0.6 eV. The transmission spectra of the metasurfaces under different Fermi levels of graphene are calculated in figure 7. Compared with the pronounced dip in the transmission spectrum of all-dielectric metasurfaces without graphene, the amplitude modulation of the asymmetric Fano transmission spectra can be observed with the Fermi level $E_F = 0.6$ eV, and much further stronger with $E_F = 0.5$ eV. Finally, the sharp resonance spectrum becomes broad and flat for the case of the undoped graphene with $E_F = 0$ eV. The absolute value of the modulation depth $\Delta T$ is employed to evaluate the modulation performance. With the results of $\Delta T = 55.08\%$, 14.79%, 0.17% for $E_F = 0$ eV, 0.5 eV and 0.6 eV, the modulation depth gradually decreases and the $Q$-factor of the resonances accordingly increases from 131.07, 646.34 to 1087.10 when the Fermi level of graphene increases. By shifting the Fermi level of graphene in the structure, the transmission amplitude...
The modulation depth can be calculated as the resonance is even switched off as the layer number reaches graphene increases at a nearly fixed resonance frequency, and of the resonance shows a rapid decline as the layer number of 25 nm in width. It is observed that the transmission amplitude metasurfaces on the layer number of graphene.

especially, when conductivity decreases with the increase of the Fermi level near infrared regime of interest, the real part of the graphene be exact, arises from the absorption effect of graphene. In the the graphene layer and the localized hot spots in the gaps, to metasurfaces originates from the strong interaction between the intrinsic absorption of graphene with the Fano­resonant all­dielectric structure, the Fano resonance strength is manipulated by changing the gap width of the resonators, shifting the Fermi level of graphene and varying the layer number of graphene. The trade­off between the field enhancement and the modulation depth upon the gap width of the resonators needs to be carefully optimized in tailoring the interaction between graphene and dielectric structure. The modulation in the transmission amplitude of Fano resonance by varying the Fermi level and the layer number of graphene further demonstrates the strong interaction between the intrinsic absorption of graphene with the electric field in the localized hot spots. This work offers great prospects for designing active and compact metade­vices such as light modulators, switches and biosensors, and the compatibility of graphene with dielectric materials would endow it with remarkable applicability for integration tech­nologies in the near future.

**4. Conclusions**

In conclusion, we symmetrically investigate the interaction between graphene with the Fano-resonant all-dielectric metasurfaces. Using silicon split resonators as the building blocks of the metasurfaces, Fano resonance with a remarkably high $Q$-factor and highly localized hot spots inside the gaps is observed. With graphene covering the dielectric structure, the Fano resonance strength is manipulated by changing the gap width of the resonators, shifting the Fermi level of graphene and varying the layer number of graphene. The trade­off between the field enhancement and the modulation depth upon the gap width of the resonators needs to be carefully optimized in tailoring the interaction between graphene and dielectric structure. The modulation in the transmission amplitude of Fano resonance by varying the Fermi level and the layer number of graphene further demonstrates the strong interaction between the intrinsic absorption of graphene with the electric field in the localized hot spots. This work offers great prospects for designing active and compact metade­vices such as light modulators, switches and biosensors, and the compatibility of graphene with dielectric materials would endow it with remarkable applicability for integration tech­nologies in the near future.

**Acknowledgments**

This work is supported by the National Natural Science Foundation of China (Grant Nos. 61775064, 11847100 and 11847132), the Fundamental Research Funds for the Central Universities (HUST: 2016YXMS024) and the Natural Science Foundation of Hubei Province (Grant Nos. 2015CFB398 and 2015CFB502).

**ORCID iDs**

Shuyuan Xiao  https://orcid.org/0000-0002-4446-6967
Tingting Liu  https://orcid.org/0000-0003-3671-2782
Xiaoyun Jiang  https://orcid.org/0000-0003-2609-6963
Zhong Li  https://orcid.org/0000-0002-2530-1323
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