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Gupta, Manoj; Singh, Ranjan

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Terahertz sensing with optimized Q/V_{eff} metasurface cavities*Manoj Gupta, and Ranjan Singh**

Dr. M. Gupta, Prof. R. Singh

Division of Physics and Applied Physics, School of Physical and Mathematical Sciences, Nanyang Technological University, 21 Nanyang Link, Singapore 637371

Dr. M. Gupta, Prof. R. Singh

Center for Disruptive Photonic Technologies, The Photonics Institute, Nanyang Technological University, 50 Nanyang Avenue, Singapore 639798

E-mail: ranjans@ntu.edu.sg**Keywords:** high Q/V_{eff} cavity, photon lifetime, sensing, mode volume, metasurface**Abstract**

Confinement of electromagnetic radiation in a subwavelength cavity is an important platform for strong light matter interaction as it enables efficient design of photonic switches, modulators and ultrasensitive sensors. Metallic metasurfaces consist of an array of planar cavities that allow easy access to confined electromagnetic modes on the surface. However, the radiative and non-radiative losses limit the quality factor (Q) of the resonantly confined mode. Therefore, metasurface designs with effectively low mode volume (V_{eff}) cavities become extremely important for enhancing the photonic density of states. Here, we experimentally demonstrate a symmetric Lorentzian resonant metasurface with lower V_{eff} as compared to asymmetric Fano resonators. Lower mode volume and optimized Q/V_{eff} metasurfaces reveal enhanced sensitivity for ultrathin analyte overlayers deposited on metasurfaces signaling enhanced light-matter interaction. Such metasurfaces with tightly confined electromagnetic modes could find wide range of applications in the development of terahertz metadevices including ultrasensitive sensors, bandpass filters, and energy-efficient modulators.

1. Introduction

Light matter interaction is one of the most vibrant research areas of increasing scientific importance and continues to grow exponentially over the coming years. These interactions are not only important for fundamental scientific research such as strong coupling regime,^[1,2] nonlinear optics,^[3,4] but also tend to be useful in developing unique applications ranging from sensing,^[5,6] switching,^[7,8] and information processing.^[9,10] Enhanced light matter interaction requires strong localization of electromagnetic energy in very small volumes, which could be engineered in subwavelength resonant structures. Resonant electromagnetic excitation is of prime importance in confining energy temporally and spatially.^[11,12] Temporal confinement is characterized by linewidth of resonance, which represents cavity photon lifetime. Spatial confinement is attributed to density of photons and depends on the resonance strength. Simultaneously achieving high spatial and temporal confinement is a continuous quest for designing low energy modulators,^[13] laser cavities,^[14] and low loss guided mode resonance filters.^[15,16] Resonant cavities with high $\frac{Q}{V_{eff}}$ ratio represent long-lasting density of photons, where Q is the quality factor of resonant excitation and V_{eff} is the effective mode volume of the cavity. The effective mode volume is calculated according to standard Purcell definition, $V_{eff} = \frac{\int_V \epsilon(r) |E(r)|^2 dV}{\max[\epsilon(r) |E(r)|^2]}$,^[17] where $\epsilon(r)$ is the dielectric constant, $|E(r)|$ is the electric field strength and V is a volume encompassing the resonator with a boundary in the radiation zone of the cavity mode. Light matter interaction is also important in realizing coupled light-matter polaritonic states, where high $\frac{Q}{V_{eff}}$ cavities have been used to access different coupling regimes of light matter interaction.^[1,18-20] For example, strong coupling regimes of light matter interactions that occur at cryogenic temperatures, could be observed at room temperature using ultralow mode volume nanocavities.^[21]

The confinement of light through subwavelength cavity enable much smaller mode volume beyond the diffraction limit.^[22] The relative squeezing of confined electromagnetic mode (V_{eff}) with respect to wavelength within cavity material $\left(\frac{\lambda_o}{n}\right)$ is represented by $\frac{V_{eff}}{\left(\frac{\lambda_o}{n}\right)^3}$, which is the normalized effective mode volume V_{eff}^N , where λ_o is the free space wavelength and n is the refractive index of medium. One can tailor the dimensions of a cavity to realize extremely small V_{eff}^N to restrict the interaction between matter and electromagnetic field. At terahertz frequencies, few electrons ultra-strong light-matter coupling has been demonstrated using nanometric split gap cavity having V_{eff}^N of 7×10^{-10} .^[23] Such extremely small cavities are usually desirable for reduced number of excitations coupled to electromagnetic field, where amplitude of resonant excitation is typically weak in nature. However, strong macroscopic response requires large active area for interaction, for which micron sized cavity with high field confinement are desired at terahertz frequencies. Metasurface composed of dielectric or metallic resonators provide such electromagnetic confinement where confined modes have been used to demonstrate perfect absorber,^[24,25] higher harmonic generation,^[3,26] sensing,^[27,28] and lasing spaser.^[29]

Metasurfaces have shown wide range of exotic potential applications, especially in enhancing matter-photon coupling. Specifically, low mode volume confinement of the electromagnetic energy in these structures have attracted enormous interest in modifying the emission properties of the quantum materials and molecular sensing applications.^[21,30] Conventional planar metallic resonator structures contain an open cavity exhibiting strong vacuum fields, which are suitable for strong and ultra-strong light-matter interaction.^[23] Additionally, the field distribution of the confined mode in extremely thin metasurface cavity takes the form of hyperbolic cosine catenary

function, which could be useful in designing and understanding of multilayered metasurface for practical applications.^[31, 32]

Metallic resonators supporting Fano resonant modes within a broad dipolar response possess high Q with large field confinement, which have been extensively used for low threshold switching, sensing and radiation loss tailoring applications.^[33-35] However, the application of such devices is limited because of the exchange interaction between the cavity modes (dipole and the Fano resonant modes), which hinders the efficient coupling of the vacuum fields to the matter excitations. Additionally, radiative and non radiative losses limit the Q factor of resonantly confined mode, therefore low V_{eff} is required to enhance $\frac{Q}{V_{eff}}$ value through innovative metasurface designs. Hence, it is highly advantageous to realize strongly confined single resonant electromagnetic mode.

In this work, we demonstrate an ‘I’ design based planar metallic metasurface platform containing micron sized cavity with optimized $\frac{Q}{V_{eff}}$ value, which possess highly sensitive, single resonant mode at 0.6 THz. We compared the performance of Lorentzian resonant ‘I’ design platform with typical asymmetric Fano resonator platform. At nearly the same frequency regime of operation, new design offers significantly small V_{eff} of $7.6 \times 10^{-8} \left(\frac{\lambda_0}{n}\right)^3$, as compared to Fano resonant metasurface with V_{eff} of $1.0 \times 10^{-7} \left(\frac{\lambda_0}{n}\right)^3$. For comparative analysis, we have taken the well-established Fano resonant platform (asymmetric double split gap resonator) because it offers much lower V_{eff} compared to other metallic resonator designs, which typically have V_{eff} value close to $10^{-4} \left(\frac{\lambda_0}{n}\right)^3$ at near-infrared and mid-infrared frequencies.^[36] We also performed the sensing experiment to demonstrate the capability of new metasurface exhibiting enhanced sensitivity for thin analyte overlayer. For 0.24 μm thick analyte layers our design shows exceptionally high

sensitivity of 18 GHz/RIU with 3 μm width of the split gap. Additionally, for similar substrate (Silicon substrate) conditions, the simulated sensitivity of cavity resonator for 4 μm thick analyte layers turns out to be around 61 GHz/RIU as compared to Fano resonator platform which has sensitivity of around 39 GHz/RIU.^[37] Realizing pure single mode cavity with large $\frac{Q}{V_{eff}}$ ratio would open a path towards realization of new nonlinear devices, ultrasensitive sensors, low threshold switching and enhanced cavity-matter coupling.

2. Discussion

The newly designed planar terahertz metasurface platform has been experimentally realized and thoroughly investigated for its low mode volume feature. **Figure 1a** shows the microscopic image of fabricated metallic pattern on 0.5 mm thick silicon (refractive index =3.42) substrate. The metasurface has been fabricated through single step lithography, followed by thermal deposition of 200 nm aluminum (Al) metal. Inset image shows the unit cell with periodicity of 75 μm x 85 μm and subwavelength micron-scale dimensions of metallic pattern. The central metallic strip is 2 μm in width, and contains 3 μm x 2 μm sized split gap at the center. Metallic patterns in unit cell are conductively coupled to neighboring unit cells. The substrate area visible from the top of unit cell, closely resemble the english alphabet ‘I’, so we address this design as ‘I-design’. The sample is excited by terahertz radiation incident normal to the plane of metasurface (Z-axis) and having its electric field polarization ($\vec{E}_x$) along metallic lines. **Figure 1b** shows experimentally measured resonance feature in transmission spectra at 0.6 THz, which is in good agreement with CST simulations. At resonance frequency, the inset in figure 1b shows simulated electric field confined in the gap of resonator. The experimentally measured Q -factor of resonance is 6, which is defined as the ratio of resonance frequency to full width at half maximum (FWHM) in resonance intensity spectrum. In order to examine the response of the confined field to the nearby dielectric

environment, we spin coated analyte (photoresist of refractive index 1.6) on the top of metallic pattern, as depicted in **Figure 1c**. The experimentally measured frequency shift for 1.5 μm thick analyte is found to be 16 GHz (figure 1d). At terahertz frequencies (0.2-1.0 THz), for similar photoresist thickness and substrate conditions, the observed frequency shift with new ‘I’ design is found to be greater than the previously reported frequency shift value (10 GHz) achieved for highly sensitive Fano design-based metamaterial platform.^[37] Therefore, we performed a comparative study to investigate the enhanced performance of ‘I’ design symmetric Lorentzian resonator over symmetry broken Fano resonator.

For detailed analysis we considered 75 μm x 75 μm unit cell of metasurface containing square shaped double split gap asymmetric resonator (Fano design) with aluminum metal strip (blue color) width of 6 μm , as shown in figure 2a. Fano design has split gap width of 3 μm , similar to that in ‘I’ design resonator (Figure 2b), in which asymmetry arises due to the shifting of bottom arm split gap by distance d from the center of resonator. CST simulations were performed for 4 μm thick analyte layer on both metasurface configurations with respect to the incoming terahertz field polarization ($\vec{E}$) depicted in **Figure 2a, b**. **Figure 2c, d** shows transmission spectra of Fano and ‘I’ design based metasurface, as refractive index (n) of analyte changes from $n=1$ (air) to $n=4$. Fano design shows two characteristic electromagnetic resonance dips; first narrow asymmetric resonance (Fano resonance) at lower frequency (0.49 THz for analyte refractive index $n=1$) and second broad symmetric resonance at higher frequency (0.7 THz for analyte refractive index $n=1$). At narrow resonance electromagnetic fields are strongly confined in the split gaps of Fano resonator, which makes metal based Fano resonator platform suitable for investigating light matter interaction at terahertz frequencies.^[38-40] As analyte refractive index is changed to $n=4$, red shift of 122 GHz is numerically observed for sharp asymmetric Fano resonance metasurface. Similar

variation in analyte refractive index shows red shift of resonance peak by 180 GHz in the ‘I’ design, which is significantly higher than the Fano design. Moreover, simulated electromagnetic field strength confined in split gap of ‘I’ design is remarkably high compared to Fano design, as shown in **Figure 2e, f**, which further establishes the enhanced efficiency of new metasurface over split ring resonator based Fano metasurface. Large field strength in split gap cavity of ‘I’ design reduces the V_{eff} of electromagnetic confinement, which enhances metasurface sensitivity. Moreover, the confined field in ‘I’ design unit cell is not limited to the vicinity of the split gap, and rather extends along the length of the metallic strips containing the split gap cavity (as shown in Figure 2f). Therefore, the surrounding region close to vicinity of central metallic strips contribute significantly towards the enhanced sensitivity of the metasurface.

Table 1. Q , V_{eff} , Q/V_{eff} and λ_o/n values at Fano resonance (for different asymmetries; $d= 5, 10, 15 \mu\text{m}$) and ‘I’ design resonance.

	Fano design (with different asymmetry, d)			‘I’ Design
	$d= 5 \mu\text{m}$	$d= 10 \mu\text{m}$	$d= 15 \mu\text{m}$	
Q factor	27.5	11	8	10
$V_{eff} = V_{eff}^N \times \left(\frac{\lambda_o}{n}\right)^3$	$40 \mu\text{m}^3$ or $1.93 \times 10^{-7} \left(\frac{\lambda_o}{n}\right)^3$	$22 \mu\text{m}^3$ or $1.0 \times 10^{-7} \left(\frac{\lambda_o}{n}\right)^3$	$31 \mu\text{m}^3$ or $1.4 \times 10^{-7} \left(\frac{\lambda_o}{n}\right)^3$	$9.5 \mu\text{m}^3$ or $7.6 \times 10^{-8} \left(\frac{\lambda_o}{n}\right)^3$
Q/V_{eff}	0.6875	0.5	0.258	1.05
λ_o/n	$591 \mu\text{m}$	$598 \mu\text{m}$	$609 \mu\text{m}$	$500 \mu\text{m}$

Further to quantify the enhanced efficiency, we did numerical $\frac{Q}{V_{eff}}$ estimations of resonantly confined electromagnetic modes in the split gaps of both designs, as depicted in **Table 1**. Comsol Multiphysics software tool was employed to perform the volume integral for V_{eff} calculation. At resonance, the confined electromagnetic mode in split gap cavity extends to about $13 \mu\text{m}$ in both directions perpendicular to the plane of metasurface, which need to be considered for mode volume

analysis. Therefore, we have performed volume integral up to distance of $30\ \mu\text{m}$ above and below the plane of unit cell, where the cross-section of 3D rectangular region is represented by the size of the unit cell. The calculated Q factor and V_{eff} of Fano design has strong dependence on the position of split gap (degree of asymmetry), whereas the position of the split gap does not effect the ‘I’ design. Numerically calculated V_{eff} of ‘I’ design is around $9.5\ \mu\text{m}^3$, compared to V_{eff} of Fano design which depending on asymmetry ranges from 22 to $40\ \mu\text{m}^3$. Since Fano and ‘I’ design resonance appears at different frequencies, therefore, we have also represented V_{eff} in terms of V_{eff}^N and $\frac{\lambda_o}{n}$ (values depicted in **Table 1**) to have a comparative estimates of V_{eff}^N , which again has relatively low value of 7.6×10^{-8} for the ‘I’ design. Further, we compared the $\frac{Q}{V_{eff}}$ values for both resonator configuration, which shows that despite having low Q factor, the new ‘I’ design shows high $\frac{Q}{V_{eff}}$ value of 1.05 , thereby accounts for enhanced efficiency compared to Fano design for which $\frac{Q}{V_{eff}}$ values lie in the range of 0.258 to 0.6875 . In the ‘I’ design, continuous metallic strip above and below the split gap cavity plays a significant role in reducing the V_{eff} of the confined electromagnetic mode. These strips enhance the overall capacitance of the metamaterial unit cell, which allows the resonating split gap cavity to store more electromagnetic energy (additional details included in *Section A* of supplementary information). Moreover, the V_{eff} number could be further improved by narrowing the capacitive split gap separation which can easily increase the $\frac{Q}{V_{eff}}$ value of the metasurface. Resonator fringing field contributes significantly to the mode volume, therefore, lowering the split gap separation beyond certain limit does not lower the mode volume drastically (additional details inculded in *Section B* of supplementary information). Due to

limited resolution of photolithography process, we fabricated samples having smallest dimensional features between 2 to 3 μm , which limited the $\frac{Q}{v_{eff}}$ value of designed metasurface.

We experimentally verified the impact of optimized $\frac{Q}{v_{eff}}$ subwavelength confinement on the sensitivity of ‘I’ design metasurface. We coated new set of samples with 0.24 μm thick layer of Silicon dioxide (SiO_2) and Germanium (Ge), due to high contrast in their refractive index. To identify the shift in resonant response, nitrogen (N_2) environment is used as the reference medium for both materials. Significant shift in resonance frequency compared to N_2 environment, could be observed in simulated (**Figure 3a**) and experimental (**Figure 3b**) transmission spectra for ~ 0.24 μm thin film coating of SiO_2 (refractive index $n=1.98$) and Ge (refractive index $n=4$). Experimentally estimated value of sensitivity from frequency shift versus refractive index plot in **Figure 3c** is found to be around 18 GHz/refractive index unit (RIU), which matches well with the simulated results (inset plot in Figure 3c). The obtained sensitivity values are significantly higher than previously demonstrated sensitivity of 6 GHz/RIU with planar toroidal metasurface based on Fano resonator platform.^[41]

Finally, we compared the sensitivity of the ‘I’ design, and Fano design for sufficiently thick analyte layer on the top of metasurface. Simulated transmission plot in **Figure 4a, b** shows the red shift in the resonance frequency with increase in the refractive index of 4 μm thick analyte layer on ‘I’ design and Fano design, respectively. The variation in frequency shifts (as shown in **Figure 4c**) appears to be linear in nature for both designs. ‘I’ design shows sensitivity of 61 GHz/RIU compared to previously reported sensitivity of 39 GHz/RIU for Fano design with 4 μm thick analyte layer.^[36] Additional comparative feature between both designs that could be highlighted in terms of resonance linewidth narrowing with increase in the analyte refractive index. **Figure 4d** shows relatively large resonance linewidth narrowing (negative slope of linear fit performed on

resonance linewidth points) in ‘I’ design compared to Fano design with increasing analyte refractive index. Therefore, effectively low mode volume in the ‘I’ design cavity acts as an efficient platform for interaction between matter and light, which tends to be better compared to existing metamaterial platforms in terahertz frequency regime with identical width of the capacitive split gap.

3. Conclusion

In conclusion, we experimentally demonstrate ‘I’ design-based terahertz metamaterial cavity featuring large electromagnetic energy confined in low mode volume that gives rise to large Q/V_{eff} in spite of lower quality factor of the metasurface. The newly designed metamaterial cavity exhibits single mode resonance feature with V_{eff}^N of 7.6×10^{-8} at 0.6 THz, resulting in enhanced sensitivity of thin analyte overlayers. Subwavelength, single mode resonant electromagnetic confinement with optimized Q/V_{eff} in metasurfaces opens an enabling platform for efficient probing of light matter interaction. The finding also highlights the importance of single mode cavity resonance with low mode volumes for ultrasensitive sensing, bandpass filters, energy-efficient photonic devices, and nonlinear effects arising from the strong light-matter interactions.

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Figure 1

Figure 1. a) Microscopic image of fabricated sample, where inset image shows the length scale (in micron) of metallic pattern ('I' design) in the unit cell. b) Simulated and experimentally measured transmission spectra of sample, with inset image shows resonant electric field confinement in the split gap at ~ 0.6 THz. c) Schematic image representing terahertz excitation of metasurface with analyte on the top. d) Experimentally measured resonance shift of 16 GHz in transmission spectra, when $1.5 \mu\text{m}$ thick analyte (refractive index=1.6) is coated on top of the sample.

Figure 2

Figure 2. Schematic image of unit cell representing a) Fano design, and b) I-design (aluminum metal is highlighted in blue color) resonator excited by terahertz electric field polarization ($\vec{E}$). Simulated transmission spectra representing frequency shift (blue dotted arrow) for c) Fano, and d) I-design metasurface, when 4 μm thick analyte of refractive index (n) is coated on top of the metasurface. Simulated resonant electric field strength and V_{eff} of confined mode in split gap of e) Fano (at 0.49 THz), and f) I-design (at 0.6 THz) at electromagnetic resonance in absence of analyte ($n=1$) on the metasurface.

Figure 3

Figure 3. a) Simulated and b) experimentally measured transmission spectra of I-design metasurface with 0.24 μm thick analyte of varying refractive index on top of the metasurface: $n=1$ (no analyte coating), $n=1.98$ (SiO₂), $n=4$ (Ge). c) Experimentally measured and simulated (inset plot) resonance frequency shift (GHz) versus refractive index (n) variation for samples coated with SiO₂ and Ge.

Figure 4

Figure 4. a, b) Simulated transmission spectra of I-design and Fano resonator based metasurface with 4 μm thick analyte of different refractive index ($n= 1, 2, 3, 4$) on top of the metasurface. c) Sensitivity of Fano and I-design metasurface depicted by frequency shift versus refractive index plot for 4 μm thick analyte layer. d) Variation in line width of resonance (I-design and Fano design) with change in refractive index of 4 μm thick analyte layer.