Design of Fano Resonators for Novel Metamaterial Applications

Thesis by
Muhammad Amin

In Partial Fulfillment of the Requirements
For the Degree of
Doctor of Philosophy

King Abdullah University of Science and Technology, Thuwal,
Kingdom of Saudi Arabia

April, 2014
The thesis of Muhammad Amin is approved by the examination committee

Committee Chairperson: Dr. Hakan Bağcı
Committee Member: Dr. Boon Ooi
Committee Member: Dr. Ying Wu
ABSTRACT

Design of Fano Resonators for Novel Metamaterial Applications

Muhammad Amin

The term “metamaterials” refers to engineered structures that interact with electromagnetic fields in an unusual but controllable way that cannot be observed with natural materials. Metamaterial design at optical frequencies oftentimes makes of controllable plasmonic interactions. Light can excite collective oscillations of conduction band electrons on a metallic nanostructure. These oscillations result in localized surface plasmon modes which can provide high confinement of fields at metal-dielectric interfaces at nanoscale. Additionally scattering and absorption characteristics of plasmon modes can be controlled by geometrical features of the metallic nanostructures. This ease of controllability has lead to the development of new concepts in light manipulation and enhancement of light-material interactions. Fano resonance and plasmonic induced transparency (PIT) are among the most promising of those. The interference between different plasmon modes induced on nanostructures generates PIT/Fano resonance at optical frequencies. The unusual dispersion characteristics observed within the PIT window can be used for designing optical metamaterials to be used in various applications including bio-chemical sensing, slow light, modulation, perfect absorption, and all-optical switching.

This thesis focuses on design of novel plasmonic devices to be used in these appli-
cations. The fundamental idea behind these designs is the generation of higher-order plasmon modes, which leads to PIT/Fano resonance-like output characteristics. These are then exploited together with dynamic tunability supported by graphene and field enhancement provided by nonlinear materials to prototype novel plasmonic devices. More specifically, this thesis proposes the following plasmonic device designs.

(i) Nano-disk Fano resonator: Open disk-like plasmonic nanostructures are preferred for bio-chemical sensing because of their higher capacity to be in contact with greater volumes of analyte. High effective refractive index required by sensing applications is achieved through the dispersion characteristics within PIT window. Higher order modes required for Fano resonance are generated through geometrical symmetry breaking by embedding a shifted and elongated cavity into a circular disk. The resulting dual band PIT can be geometrically tuned by varying the cavity’s width and rotation angle.

(ii) Tunable Terahertz Fano resonator: The possibility to dynamically tune graphene’s conductivity has made it an attractive choice over conventional noble metals to generate surface plasmon modes at Terahertz frequencies. Subsequently, a polarization-independent and dynamically tunable hybrid gold-graphene structure is designed to achieve PIT/Fano resonance by allowing graphene and metallic plasmon modes to interfere. The effective group index of the resulting resonator is found to be very high ($n_g > 1400$, several times higher than all previously reported PIT devices) within the PIT window. Dynamic tunability achieved through a gate voltage applied to graphene suggests applications in switching.

(iii) Tunable Terahertz Fano absorber: Many photonic and optical devices rely on their ability to efficiently absorb an incoming electromagnetic field. The absorption in atomically thin graphene sheet is already very high i.e., “2.3%” per
layer. However, considering its atomic thickness graphene sheet remains practically transparent to Terahertz waves. The proposed absorber design makes of an asymmetrically patterned graphene layer that supports higher order plasmon modes at Terahertz frequencies. Several of these patterned layers backed by dielectric substrates are stacked on top of each other followed by reflector screen. The dynamically controllable resonances from each graphene layer and the spacing between them are fine tuned to achieve a large bandwidth of 6.9 Terahertz (from 4.7 to 11.6 Terahertz) for over 90% absorption, which is significantly higher than that of existing metallic/graphene absorbers.

(iv) Three state all-optical switch: The plasmonic resonances are extremely sensitive to dielectric properties of the surrounding medium. A slight change in the dielectric constant near the metal surface results in a significant change in the plasmonic resonance. This sensitivity is enhanced in the presence of a nonlinear change in the dielectric constant. To make use of this effect, Fano resonator is used in conjunction with a Kerr nonlinear material. The resulting resonator exploits multiple (higher order) surface plasmons to generate a multi-band tri-stable response in its output. This cannot be obtained using existing nonlinear plasmonic devices that make use of single mode Lorentzian resonances. Multi-band three-state optical switching that can be realized using the proposed resonator has potential applications in optical communications and computing.
ACKNOWLEDGEMENTS

I am thankful to my supervisor Dr. Hakan Bağcı for giving me opportunity to work with him. He believed in my success from the first day and gave me the confidence to undertake this new domain of research. He provided a continuous dedicated support and guidance without which this research work would not have been successful. I am extremely thankful for the time, help, motivation and facilities he provided me during my PhD studies. I am grateful to my friend Dr. Mohamed Farhat for his time, motivation and taking personal interest in assisting me to do such a valuable research work in this field. I would also like to thank my thesis committee Dr. Boon Ooi and Dr. Ying Wu for taking their precious time attending my thesis defense. I would like to thank Dr. Carsten Rockstuhl for providing feedback on my thesis. I would also like to thank Dr. Anand Srinivasan, Dr. Naeem Shahid, Dr. Shagufta Noreen, Dr. Bruce Sinclair and Dr. Arshad Ali for their guidance during my academic career. My thanks also go to all my friends in the lab from students to postdocs Abdulla Desmal, Ismail Enes Uysal, Sadeed Bin Sayed, Ali Imran, Ozum Asirim, Yasser Khan, Dr. Kostyantyn Sirenko, Dr. Mohamed A. Salem, Dr. Ahmed Al-Jarro, Dr. Huseyin Arda Ülkü and Dr. Yifei Shi for their continuous support whenever I needed them.

My deepest gratitude goes to my family for their support throughout my life. I want to thank my siblings Atif, Bushra, Kashif and Yasir for providing me guidance ever since my childhood. I want to thank my wife Maham Sarfraz for taking care and helping me during difficult times. Finally, I want to thank my parents specially my father who is the real source of inspiration for my life. I need them in my life today much more than from yesterday and I could only wish to serve them better.
<table>
<thead>
<tr>
<th>Section</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>Examination Committee Approval</td>
<td>2</td>
</tr>
<tr>
<td>Copyright</td>
<td>3</td>
</tr>
<tr>
<td>Abstract</td>
<td>4</td>
</tr>
<tr>
<td>Acknowledgements</td>
<td>7</td>
</tr>
<tr>
<td>List of Figures</td>
<td>12</td>
</tr>
<tr>
<td>List of Tables</td>
<td>17</td>
</tr>
<tr>
<td>1 Introduction</td>
<td>18</td>
</tr>
<tr>
<td>1.1 Fano resonance</td>
<td>22</td>
</tr>
<tr>
<td>1.1.1 Designer dispersion via plasmonic Fano resonance</td>
<td>22</td>
</tr>
<tr>
<td>1.2 Scope of thesis</td>
<td>24</td>
</tr>
<tr>
<td>2 A dual-band nano-disk Fano resonator</td>
<td>27</td>
</tr>
<tr>
<td>2.1 Introduction</td>
<td>27</td>
</tr>
<tr>
<td>2.2 Design details and results</td>
<td>31</td>
</tr>
<tr>
<td>2.2.1 Disk with concentric elongated cavity</td>
<td>31</td>
</tr>
<tr>
<td>2.2.2 Disk with shifted elongated cavity</td>
<td>33</td>
</tr>
<tr>
<td>2.2.3 Disk with shifted and rotated elongated cavity</td>
<td>38</td>
</tr>
<tr>
<td>2.3 Methods</td>
<td>42</td>
</tr>
<tr>
<td>2.3.1 RLC circuit model</td>
<td>42</td>
</tr>
<tr>
<td>2.3.2 Simulation parameters</td>
<td>46</td>
</tr>
<tr>
<td>2.4 Discussion and possible limitations</td>
<td>47</td>
</tr>
<tr>
<td>2.5 Summary</td>
<td>47</td>
</tr>
<tr>
<td>3 A dynamically tunable Fano resonator</td>
<td>49</td>
</tr>
<tr>
<td>3.1 Introduction</td>
<td>49</td>
</tr>
<tr>
<td>3.2 Design details and results</td>
<td>51</td>
</tr>
<tr>
<td>Section</td>
<td>Title</td>
</tr>
<tr>
<td>---------</td>
<td>---------------------------------------------------------</td>
</tr>
<tr>
<td>3.2.1</td>
<td>Physical mechanism</td>
</tr>
<tr>
<td>3.2.2</td>
<td>Proof of concept via numerical experiments</td>
</tr>
<tr>
<td>3.3</td>
<td>Applications</td>
</tr>
<tr>
<td>3.4</td>
<td>Material models</td>
</tr>
<tr>
<td>3.5</td>
<td>RLC analytic model</td>
</tr>
<tr>
<td>3.6</td>
<td>Discussion and possible limitations</td>
</tr>
<tr>
<td>3.7</td>
<td>Summary</td>
</tr>
<tr>
<td>4.1</td>
<td>Introduction</td>
</tr>
<tr>
<td>4.2</td>
<td>Design details and results</td>
</tr>
<tr>
<td>4.2.1</td>
<td>Design</td>
</tr>
<tr>
<td>4.2.2</td>
<td>Patterned graphene layer</td>
</tr>
<tr>
<td>4.2.3</td>
<td>One-layer graphene absorber</td>
</tr>
<tr>
<td>4.2.4</td>
<td>Two-layer graphene absorber</td>
</tr>
<tr>
<td>4.2.5</td>
<td>Three-layer graphene absorber</td>
</tr>
<tr>
<td>4.3</td>
<td>Discussion and possible limitations</td>
</tr>
<tr>
<td>4.4</td>
<td>Summary</td>
</tr>
<tr>
<td>5.1</td>
<td>Introduction</td>
</tr>
<tr>
<td>5.2</td>
<td>Design details and results</td>
</tr>
<tr>
<td>5.2.1</td>
<td>Design</td>
</tr>
<tr>
<td>5.2.2</td>
<td>Linear simulations</td>
</tr>
<tr>
<td>5.2.3</td>
<td>Nonlinear simulations</td>
</tr>
<tr>
<td>5.3</td>
<td>Discussion and possible limitations</td>
</tr>
<tr>
<td>5.4</td>
<td>Summary</td>
</tr>
<tr>
<td>6.1</td>
<td>Summary</td>
</tr>
<tr>
<td>6.2</td>
<td>Future research work</td>
</tr>
<tr>
<td>6.2.1</td>
<td>Acoustic Fano resonance</td>
</tr>
<tr>
<td>6.2.2</td>
<td>Polarization Independent Absorption</td>
</tr>
<tr>
<td>6.2.3</td>
<td>Enhancement of nonlinearity using plasmonic near-field</td>
</tr>
<tr>
<td>6.2.4</td>
<td>Non-reciprocity of light</td>
</tr>
<tr>
<td>6.2.5</td>
<td>Effective medium for describing asymmetric metamaterial response</td>
</tr>
</tbody>
</table>
# LIST OF FIGURES

<table>
<thead>
<tr>
<th>Figure</th>
<th>Description</th>
<th>Notes</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.1(a)</td>
<td>Metamaterial tree of knowledge (MTK) showing progress and future of metamaterial research. The originally forbidden fruit of negative index is now ripped (red apples). Studies on controlling spatial distribution and dispersion characteristics of EM fields are flourishing (yellow apples). The emerging directions are sensing, amplifying, switchable, nonlinear, and quantum metamaterials (green apples). Reprinted with permission from AAAS</td>
<td>20</td>
</tr>
<tr>
<td>2.1</td>
<td>Description of the incident electromagnetic field and the schematic views of the circular disk with (a) the concentric elongated cavity, (b) the shifted elongated cavity, and (c) the shifted and rotated elongated cavity.</td>
<td>29</td>
</tr>
<tr>
<td>2.2</td>
<td>Extinction CS spectrum of the circular disk with the concentric elongated cavity. The geometry parameters shown in Fig. 2.1(a) and the height of the structure are $D = 100,\text{nm}$, $L = 65.5,\text{nm}$, $W = 35,\text{nm}$, and $H = 10,\text{nm}$ respectively. The inset shows the charge distribution on the structure at 762 nm, marked with the blue dot on the plot. All the charges in the color plot are normalized between 1 and -1 (red and blue).</td>
<td>33</td>
</tr>
<tr>
<td>2.3(a)</td>
<td>Extinction CS spectrum of the circular disk with the shifted elongated cavity. The geometry parameters shown in Fig. 2.1(b) and the height of the structure are $D = 100,\text{nm}$, $L = 65.5,\text{nm}$, $W = 35,\text{nm}$, $O = 15.25,\text{nm}$, and $H = 10,\text{nm}$ respectively. The insets show the charge distributions on the structure at 656 nm (marked with the green dot on the plot), 696 nm (marked with the red dot), and 784 nm (marked with the blue dot). (b) Amplitude of the net dipole moment along the $x$-axis. (c) Extinction spectrum of the structure without the “wire”. The inset shows the charge distribution on the structure at 720 nm (marked with the blue dot on the plot).</td>
<td>34</td>
</tr>
</tbody>
</table>
2.4 Tunability of the design with the circular disk and the shifted elongated cavity. (a) Extinction CS spectrum of the design with the cavity filled with silica (refractive index $n = 1.5$). (b) Extinction CS spectra of the designs where the cavity’s width is changed from $W = 20$ nm to $W = 45$ nm with a step of 5 nm while the other parameters are $D = 100$ nm, $L = 65.5$ nm, $O = 15.25$ nm, and $H = 10$ nm.

2.5 (a) Extinction CS spectrum of the circular disk with the shifted and rotated elongated cavity. The geometry parameters shown in Fig. 2.1(c) and the height of the structure are $D = 100$ nm, $L = 65.5$ nm, $W = 35$ nm, $O = 15.25$ nm, $\theta = 40^\circ$, and $H = 10$ nm, respectively. The insets show the charge distribution on the structure at 622 nm (marked with the green dot on the plot), 674 nm (marked with the red dot), 788 nm (marked with the blue dot), 904 nm (marked with the cyan dot), and 1020 nm (marked with the black dot) (b) Amplitude of the net dipole moment along the $x$-axis.

2.6 Tunability of the design with the circular disk and the shifted and rotated elongated cavity. Extinction spectra of the designs where the cavity’s rotation angle is changed 10° to 90° with a step of 20° while the other parameters are $D = 100$ nm, $L = 65.5$ nm, $O = 15.25$ nm, and $H = 10$ nm.

2.7 Comparison between the rotation of cavity and disk around their respective centers for $\theta = 90^\circ$.

2.8 (a) Description of the RLC circuit that supports three resonances. (b) Normalized spectra of $P$ for the circuit with $\gamma_1 = 21.76$ THz, $\gamma_2 = 23.03$ THz, $\omega_1 = 446.98$ THz, $\omega_2 = 397.19$ THz, $\Omega_{12} = 168.50$ THz, and $\Omega_{13} = \Omega_{23} = 0$, and the extinction CS for the design with $D = 100$ nm, $W = 35$ nm, $L = 65.5$ nm, $O = 15.25$ nm, and $H = 10$ nm. (c) Normalized spectra of $P$ for the circuit with $\gamma_1 = 27.32$ THz, $\gamma_2 = 25.52$ THz, $\gamma_3 = 18.23$ THz, $\omega_1 = 464.29$ THz, $\omega_2 = 382.14$ THz, $\omega_3 = 321.49$ THz, $\Omega_{12} = 188.34$ THz, $\Omega_{13} = 125.77$ THz, and $\Omega_{23} = 145.20$ THz, and the extinction CS for the design with $D = 100$ nm, $W = 35$ nm, $L = 65.5$ nm, $O = 15.25$ nm, $H = 10$ nm, and $\theta = 40^\circ$.

3.1 (a) Top view of the unit cell with dimensions. (b) Cross section view and the normally incident excitation. (c) Doubly periodic array of the unit cell and the normally incident excitation.
3.2 (a) Transmittance of only the gold frame. $S_1 = 5.5 \, \mu \text{m}$ and $\varepsilon_d = 3.5$. SPP is marked as $D_1$. (b) Transmittance of only the graphene patch for different values of $\mu_c$. $S_2 = 1.6 \, \mu \text{m}$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\varepsilon_d = 3.5$. SPP is marked as SPP $D_2$. Transmittance of the resonator with both the gold frame and the graphene patch. $S_1 = 5.5 \, \mu \text{m}$, $S_2 = 1.6 \, \mu \text{m}$, $\varepsilon_d = 3.5$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500 \, \text{meV}$. (c) Amplitude and (d) phase.

3.3 (a) Surface charge distributions on the unit cell computed at frequency points I, II, III, and IV corresponding to the frequencies: 5.3, 7.7, 8.35 and 9 THz. $S_1 = 5.5 \, \mu \text{m}$, $S_2 = 1.6 \, \mu \text{m}$, $\varepsilon_d = 3.5$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500 \, \text{meV}$. The color scale for the positive and negative surface charges are normalized between (-1 and 1). (b) Same as in (a) but for the distribution of the norm of the magnetic field in the plane of the unit cell x-y.

3.4 (a) Transmittance of the resonator with $S_1 = 5.5 \, \mu \text{m}$, $\varepsilon_d = 3.5$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500 \, \text{meV}$ for various values of $S_2$. The transmittance of only the gold frame with $S_1 = 5.5 \, \mu \text{m}$ is plotted as a reference in thin blue line. (b) Transmittance of the resonator with $S_2 = 1.6 \, \mu \text{m}$, $\varepsilon_d = 3.5$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500 \, \text{meV}$ for various values of $S_1$. The transmittance of only the gold frame with $S_1 = 6 \, \mu \text{m}$ is plotted as a reference in thin blue line. (c) Transmittance of the resonator with $S_1 = 5.5 \, \mu \text{m}$, $S_2 = 1.6 \, \mu \text{m}$, $\varepsilon_d = 3.5$, and $\mu_c = 1500 \, \text{meV}$ for various values of $\mu$. (d) Transmittance of the resonator with $S_1 = 5.5 \, \mu \text{m}$, $S_2 = 1.6 \, \mu \text{m}$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500 \, \text{meV}$ for various values of $\varepsilon_d$.

3.5 (a) Transmittance of the resonator with $S_1 = 5.5 \, \mu \text{m}$, $S_2 = 1.6 \, \mu \text{m}$, $\varepsilon_d = 3.5$, and $\mu = 10,000 \, \text{cm}^2/\text{Vs}$ for various values of $\mu_c$ between 500 meV and 1500 meV. (b) Same as in (a) but for the phase of the transmission. The dashed white lines highlight the plasmonic EIT-like zone.

3.6 Switching applications: (a) Transmittance as function of $\mu_c$ for different values of the operation frequency: 7.1, 7.7, 7.94 and 8.22 THz. $S_1 = 5.5 \, \mu \text{m}$, $S_2 = 1.6 \, \mu \text{m}$, $\varepsilon_d = 3.5$, and $\mu = 10,000 \, \text{cm}^2/\text{Vs}$. (b) Same as in (a) but for the phase of transmission.
3.7 Retrieved (a) effective refractive index $n_e$ and (b) effective group index $n_g$ versus frequency. $S_1 = 5.5$ µm, $S_2 = 1.6$ µm, $\varepsilon_d = 3.5$, $\mu = 10,000$ cm$^2$/Vs, and $\mu_c = 1500$ meV.

3.8 Schematics of the three-loop RLC circuit. Two-loop circuit is obtained by removing the third loop by short-circuiting $C_{13}$ and $C_{23}$.

4.1 The schematic diagram of the proposed absorber with three layers of graphene.

4.2 Description of the transmission line model for the multilayered absorber.

4.3 The graphene unit cell with an asymmetric void with its dimensions.

4.4 (a) Transmittance, reflectance, and absorption of a single layer of patterned graphene for $\mu_c = 1000$ eV and $\mu = 10,000$ cm$^2$/Vs. (b) Normalized surface charge density distribution on the unit cell at the frequency points identified on the curve. (c) Transmittance and (d) reflectance spectra of the patterned graphene layer for varying values of $\mu_c$. The color bar represents the value of transmittance in (c) and reflectance in (d).

4.5 (a) Absorption spectra of the one-layer design with varying values of $d_1$ and various values of $\mu_c$. (b) Absorption spectra of the one-layer design with varying values of $\mu_c$ and various values of $d_1$. The color bar represents the value of absorption. (c) Absorption of the one-layer design with $\mu_c = 500$ meV and $d_1 = 100$ µm exhibiting multiple resonances due to smaller $\text{FSR}= 0.95 \text{THz}$.

4.6 (a) Absorption spectra of the one-layer design with varying values of $d_1$ and various values of $\mu$. The color bar represents the value of absorption. (b) Relationship between the absorption maximum and the bandwidth of 90% absorption as a function of $\mu$. (c) The absorption spectra of the one-layer design with $\mu = 1000$ cm$^2$/Vs and $d_1 = 5$ µm.

4.7 (a) Absorption spectra of the two-layer design with (a) varying values of $d_1$ and various values of $d_2$ and (b) varying values of $d_2$ and various values of $d_1$. The color bar represents the value of absorption in (a) and (b).

4.8 FOM of the two-layer design as a function of $d_1$ and $d_2$. (b) The absorption spectra of the two-layer design with $d_1 = 0.5$ µm and $d_2 = 5.45$ µm. The color bar represents the absolute value of FOM.
4.9 The absorption spectra of the three-layer design with \( d_1 = 0.67 \mu m, d_2 = 0.5 \mu m, \) and \( d_3 = 4.78 \mu m. \) 

5.1 (a) A example of 8B/6T encoding that uses three states to describe the binary data \( \text{[2]} \). (b) Schematic diagram of a three-state logic device and its truth table. The output gate supports a high impedance state in addition to the 0 and 1 logic levels \( \text{[3]} \). (c) Example use of a three-state logic gate where several devices share a single bus waveguide.

5.2 Schematic of the proposed resonator. The gap between the gold frame and the rod is highlighted in red color.

5.3 Gap electric field enhancement \( |E_g|/|E_0| \) computed at various values of \( \varepsilon_g \) at a band of frequencies between 175 THz and 500 THz. Insets show normalized surface charge density induced on the resonator surface at three different frequencies.

5.4 An example of how the graphical method is used for computing the nonlinear response of the resonator. Frequency is 410 THz and only \( |E_g| \varepsilon_g \) curves for \( I_0 = 19.5 \text{ MW/cm}^2 \) and \( I_0 = 3.74 \text{ GW/cm}^2 \) are plotted for demonstration. The intersection points on the graph represent the solution of the nonlinear simulation.

5.5 Extinction CS spectrum of the resonator with nonlinear \( \varepsilon_g = \varepsilon_L + \chi^{(3)} |E_g|^2 \), \( \varepsilon_L = 2.52 \), \( \chi^{(3)} = 6.72 \times 10^{-18} \text{ m}^2/\text{V}^2 \) and with linear \( \varepsilon_g = 2.52 \), which is computed for \( I_0 = 0.22 \text{ GW/cm}^2 \) and \( I_0 = 21 \text{ W/cm}^2 \), respectively.

5.6 Near-field response of the resonator with nonlinear permittivity \( \varepsilon_g = \varepsilon_L + \chi^{(3)} |E_g|^2 \), \( \varepsilon_L = 2.52 \), \( \chi^{(3)} = 6.72 \times 10^{-18} \text{ m}^2/\text{V}^2 \). \( \varepsilon_g \) as a function of \( I_0 \) at (a) 410 THz. Extinction CS as a function of \( I_0 \) at (b) 410 THz.

5.7 Near-field response of the resonator with nonlinear permittivity \( \varepsilon_g = \varepsilon_L + \chi^{(3)} |E_g|^2 \), \( \varepsilon_L = 2.52 \), \( \chi^{(3)} = 6.72 \times 10^{-18} \text{ m}^2/\text{V}^2 \). \( \varepsilon_g \) as a function of \( I_0 \) at (a) 498 THz. Extinction CS as a function of \( I_0 \) at (b) 498 THz.

5.8 (a) Schematic of the proposed resonator’s tri-stable output. Stable branches are labeled as state 1, 2, and 3, within the tri-stability region. (b) State flow diagram of tri-stable system’s output. All transitions from one state to another are accompanied by the required changes in the input intensity level. (c) A schematic device model of the cascaded VCSEL controlling the input intensity of a nonlinear resonator with three-state output.
LIST OF TABLES

3.1 Parameters of the RLC circuit model representing the Fano resonator with $S_1 = 5.5 \, \mu m$, $S_2 = 1.6 \, \mu m$, $\varepsilon_d = 3.5$, and $\mu = 10,000 \, cm^2/Vs$ for various values of $\mu_c$ between 500 meV and 1500 meV. Units of $\omega_1$, $\omega_2$, $\omega_3$, $\Omega_{12}$, $\Omega_{13}$, and $\Omega_{23}$ are (meV) while the units of $\varphi_1$ and $\varphi_2$ are (mV/H). .......................................................... 67

4.1 Comparison between bandwidths of 90% absorption at THz frequencies. Studies marked with * describe multiple bands of absorption above 90%. .......................................................... 73

5.1 Switching power and contrast at various threshold switching levels [Figs. 5.6(b) and 5.7(b)]. .......................................................... 102
Chapter 1

Introduction

The theory of Negative Index Medium (NIM) was originally described by Victor Veselago in 1968 [4]. His hypothesis could not be verified experimentally since materials with negative permeability were not available at that time. Later in 2000, John Pendry made the first ever practical demonstration of an NIM using split ring resonators [5, 6], which are often accepted as the first group of metamaterials since their response to electromagnetic (EM) fields is not observed with naturally occurring materials. The word “meta” means beyond and hence the term “metamaterial” refers to beyond conventional materials. Since their initial realization, metamaterials have become the topic of many emerging research directions, which are not only restricted to NIM design [7]. The unusual dispersion characteristics of metamaterials are typically achieved using carefully designed intricate and complicated geometries [8]. These engineered metamaterials can manipulate EM fields that cannot be realized by conventional means.

Usually, metamaterials are composed of meta-atoms/unit cells, in a way similar to the natural matter being composed of atoms. The unit cells, which are much smaller than the wavelength of excitation, are periodically arranged in the form of a lattice to constitute the metamaterial. As expected, the effective medium parameters of such structures depend largely on the properties of the materials and the geometrical shape used in the design of the unit cell as well as their specific periodic arrangement. Unit
cells of many metamaterials that are designed to operate at optical frequencies are made of metals (gold, silver, copper, etc.) and dielectric materials (silicon, polymers, polyimide, etc.) and are located on dielectric substrates \[9\]. Upon excitation with an external EM field, Surface Plasmon Polaritons (SPPs) are generated in the vicinity of the metal/dielectric surfaces. These SPPs are the collective oscillations of conduction electrons in response to the field incident on the structure. For metal nanoparticles with skin depth comparable to the particle size, this response arises in the form of Localized Surface Plasmons Polaritons (LSPPs) \[10\]. Plasmonics is the study of SPPs and LSSPs and their interactions with materials. Because of their unusual dispersion characteristics at optical frequencies, plasmonic structures are the prime candidates for designing optical/high-frequency metamaterials \[7\].

The growing fields of plasmonics and metamaterials are finding new research directions in various areas of engineering and applied physics [Fig. 1.1] \[1\]. Metamaterials are expected to have impact in an entire range of technologies, where EM field-material interaction is utilized to design new devices \[11\]. A comprehensive list of topics in this field of research would be too long to be included here \[11\]. Therefore, a shorter list of more fundamental and challenging topics is presented:

(i) **Optical cloaking**: A cloak of invisibility is a theme that is inspired by fiction. Improved fabrication capabilities allowing better control of metamaterials’ unusual properties (required by transformational optics) have rendered cloaking possible. Carefully tailoring the permittivity and permeability of a medium surrounding an object, one can guide the incident light around it and make the object virtually invisible to external observers \[12\].

(ii) **Super lens**: A thin slab composed of NIM is demonstrated to have imaging properties beyond the diffraction limit \[13\]. The NIM-slab reconstructs the image of an object in the EM near field. Therefore, both the propagating and evanescent fields contribute to the image increasing the resolution drastically.
Figure 1.1: (a) Metamaterial tree of knowledge (MTK) showing progress and future of metamaterial research. The originally forbidden fruit of negative index is now ripped (red apples). Studies on controlling spatial distribution and dispersion characteristics of EM fields are flourishing (yellow apples). The emerging directions are sensing, amplifying, switchable, nonlinear, and quantum metamaterials (green apples). Reprinted with permission from AAAS [1].
(iii) **Sensing**: Characteristics of SPPs generated on structured metasurfaces (surface analogue of bulk metamaterials) are extremely sensitive to the changes in the surrounding medium’s refractive index. Therefore, molecular binding events of a biological or chemical analyte (substance under test) within the near field region of SPPs can be efficiently detected [14].

(iv) **Slow light**: In contrast to conventional light trapping techniques that exploit cavity resonators, highly dispersive propagation on metasurfaces can be used to achieve significant enhancement of field-material interactions [15].

(v) **Photovoltaic cell**: New light trapping methods designed to increase absorption in solar cells include the use of metallic nanostructures to localize light [16]. Strong interaction of nanoparticles with light provides efficient absorption in the active layer and increases the overall efficiency of the solar cell.

Rapid progress in the research field of metamaterials has made them very attractive for emerging commercial technologies [17]. The applications of metamaterials are intended for industrial sectors such as telecommunications, electronics, clean energy, health and defense, etc. The unique properties of optical/plasmonic metamaterials provide efficient mechanisms to control light at the nanoscale, therefore have tremendous potential to be useful components of many nano-photonic devices and systems [17]. This potential can be fully exploited only through the success of cutting-edge research in developing novel cost-effective, reliable, and feasible plasmonic metamaterials. To this end, this thesis focuses on developing new plasmonic metamaterials and describes their possible applications in slow light, sensing, and switching domains [Fig. 1.1]. The fundamental idea behind these novel designs is to use Fano resonance and electromagnetically induced transparency to obtain the desired dispersion characteristics. These characteristics are then exploited together with dynamic tunability supported by graphene and field enhancement via nonlinear materials to prototype
metamaterials/plasmonic devices for applications mentioned above.

1.1 Fano resonance

Electromagnetically Induced Transparency (EIT) is essential in creating designer dispersion metamaterials envisioned in Fig. 1.1. Concepts of EIT and Fano resonance were originally discovered in the context of quantum mechanics [18]. Resonance can be described as the tendency of a system to oscillate at higher amplitude at certain frequencies. The spectral lineshape of such oscillations were originally explained by the symmetrical Lorentzian function, which was considered to be the default lineshape for all resonances. Ugo Fano, in 1961, for the first time, explained the unconventional asymmetric lineshape observed in some resonant scattering systems [19]. Compared to Lorentzian lineshape, the Fano lineshape (named after its inventor) is due to the quantum interference of a discrete state with a continuum state, and exhibits an asymmetric profile. It should be noted here that the same interference effects are observed in classical systems of coupled mass-spring oscillators, which are used to describe damped oscillations in mechanical systems [20, 21].

The EIT renders the medium transparent to EM fields within a narrow range of frequencies around the absorption line. EIT is often observed together with Fano resonance and generated when a narrowband discrete state destructively interferes with a broader continuum. Typically the resulting spectrum has the Fano lineshape. High dispersion characteristics are also observed within the EIT window.

1.1.1 Designer dispersion via plasmonic Fano resonance

Recently, it was suggested that EIT and Fano resonance could be generated at optical frequencies using plasmonic metamaterials [15]. Plasmonic Fano resonance is generated when two plasmon modes interfere with each other. The out-of-phase cou-
pling between the modes (destructive interference) leads to plasmonic equivalent of EIT or Plasmon Induced Transparency (PIT). The unusual dispersion characteristics observed within the EIT window can be used for realizing the designer dispersion metamaterial systems envisioned in Fig. 1.1.

The PIT could be obtained via interference of either anti-parallel dipolar SPPs or bright dipolar SPPs with higher order ones all induced on metal-dielectric interfaces [22, 23, 24]. When the structure is electrically small and symmetric with respect to the incident field’s polarization and/or direction of propagation, higher order modes cannot be excited. One can increase the electrical size of the structure (at the cost of ease of tunability) or “break” the structural symmetry to permit the incident field’s energy to couple to the higher order modes [25, 26]. The additional higher order mode enables the (destructive) interference effect required for the PIT.

Symmetry breaking has been proven useful in excitation of higher order modes to generate plasmonic Fano resonators for various nanostructures constructed from shells [26, 27, 28, 29, 30], disks [31, 32, 33, 34], cross [35, 36], dimer [37, 38], and split rings [39]. Symmetry breaking on nano dimer and nano-emitter systems supported higher order dipole and quadrupole resonances [40, 41]. Fano resonance has been generated using dipole and quadrupole modes with substrate mediated symmetry breaking effect on cubic nanoparticles [42]. Other examples of symmetry breaking methods include utilizing conductive coupling between a theta-shaped ring rod and the wall of the ring enclosing it [43] and removing a wedge slice from a metallic nanodisk [44].

Fano resonance and PIT have become topics of interest due to their promising applications in light manipulation including filtering, highly dispersive propagation (slow light) [45], bio- and chemical sensing [45, 46, 47] and optical switching [48]. Drastic slowing of light around the narrow PIT band results in enhanced light-matter interactions inside the Fano metamaterial. This highly dispersive and low-loss prop-
agitation can be used to achieve significant enhancement of nonlinear optical processes \cite{49, 50}.

1.2 Scope of thesis

The scope of the work presented in thesis is to attempt to solve some of the open problems in the field of plasmonic Fano resonators/metamaterial design. More specifically, the thesis focuses on the following novel plasmonic devices:

(i) **Nano-disk Fano resonator**: Metamaterials exploiting the Fano resonance and EIT/PIT phenomena provide a great platform to accomplish light manipulation at the nanoscale. They are more competitive than previously adopted approaches that exploit unusual dispersion characteristics observed with photonic crystals \cite{51}, waveguides \cite{52, 53, 54, 55, 56}, defect cavities \cite{57}, etc. In recognition of the significance of optical sensing in open ring-like structures \cite{58}, a multi-band Fano resonator composed of a single metal piece only is designed \cite{59}. In this novel design, two distinct higher order modes are generated through symmetry breaking. These narrowband modes interfere with the original dipole mode and generate dual EIT bands.

(ii) **Tunable Terahertz Fano resonator**: There is an increasing interest in the use of graphene instead of metals in plasmonic device designs since its conductivity can be dynamically controlled. As discussed above, the symmetry breaking is often used to design Fano resonators through the excitation of higher order SPPs \cite{15, 26, 24}. However, it leads to polarization dependent response. Symmetric designs do not suffer from this drawback. To this end, a hybrid gold-graphene resonator capable of generating highly dispersive PIT effects at Terahertz frequencies is proposed \cite{60}. The destructive interference between the narrow- and broadband dipolar surface plasmons, which are induced respec-
tively on the surfaces of the graphene patch and the gold frame, leads to the
PIT. The response of the metamaterial is polarization independent and its spec-
tral features can be controlled by a gate voltage applied to the graphene patch.
Additionally, effective group index of the device is retrieved and is found to
be very high within the PIT window suggesting its potential use in slow light
applications.

(iii) **Tunable Terahertz Fano absorber**: Many photonic and optical devices,
including detectors, sensors, solar cells, and thermal emitters, rely on their abil-
ity to efficiently absorb an incoming EM field [61]. Many existing THz-wave
absorber designs use graphene layers as their building block [62, 63, 64, 65].
This can be attributed to the fact that a graphene layer supports SPPs at
THz frequencies and at the SPP resonance frequencies, absorption is signifi-
cantly increased. Furthermore, these frequencies can be dynamically tuned via
biasing the graphene layer. For this purpose a patterned graphene metasur-
face based plasmonic absorber is designed to provide “almost” perfect absorp-
tion at a broadband of THz frequencies [66]. This wide band of absorption is
achieved by (i) asymmetrically patterning the graphene metasurfaces to support
higher order surface plasmon modes that destructively interfere with the dipoi-
lar mode and generate electromagnetically induced absorption, (ii) stacking up
these metasurfaces backed-up with dielectric substrates on top of each other,
(iii) biasing each metasurface at a different gate voltage, and (iv) finally in-
creasing the Graphene’s damping factor. Following these guidelines, bandwidth
of 90% absorption of a three-layer design is increased to 6.9 THz (from 4.7 to
11.6 THz), which is significantly wider than that of existing metallic/graphene
absorbers.

(iv) **Three state all-optical switch**: Finally, the goals identified by the nonlin-
ear and switchable metamaterials in MTK [Fig. 1.1] motivated the design of a three state memory and switch using plasmonic multi-stability. Localized field amplification on plasmonic structures provides a mechanism for enhancing the effect of nonlinearity in material properties [50]. Materials with Kerr nonlinearity have previously been used in loading plasmonic waveguides to construct ultrafast optical switches [67, 68, 69, 70, 71]. The significant improvements that come with using three-state switches (compared to their two-state counterparts) for communications and computing in the field of digital electronics have been well-understood [2, 3]. They not only increase the data rate of a communication system but also help to provide the additional “enable” input responsible for connecting or isolating the device output from the rest of the system, which cannot be achieved with gates that support standard two-state output. For this purpose we design a nonlinear plasmonic resonator for three-state all-optical switching at frequencies including near infrared and lower red parts of the spectrum [72]. The tri-stable response required for three-state operation is obtained by enhancing nonlinearities of a Kerr medium through multiple (higher order) plasmons excited on resonators metallic surfaces. Multi-band three-state optical switching that can be realized using the proposed resonator has potential applications in optical communications and computing.

In the remainder of the thesis, these novel plasmonic device designs benefiting from dispersion characteristics that come with Fano resonance/PIT are detailed in separate chapters. Chapters 2, 3, 4 and 5 focus on nano-disk resonator, tunable hybrid graphene-gold Fano resonator, tunable multi-layer graphene absorber, and three state plasmonic switch respectively. Chapter 6 draws some conclusions and briefly describes extensions of the work proposed in this thesis together with several future research directions.
Chapter 2

A dual-band nano-disk Fano resonator

2.1 Introduction

It is well known that nanostructures constructed using metallic particles are capable of supporting surface plasmon modes with resonance frequencies in the visible spectrum [73, 74]. These modes are simply collective oscillations of conduction electrons excited by electromagnetic field incident on the structure. When the structure is electrically small, i.e., its largest dimension is sub-wavelength, the optical properties of these plasmon modes depend almost exclusively on the specific shape of the structure [17]. This allows for easy tuning of the plasmon modes’ resonance frequency, localized field amplitudes, quality factor, and line-width via only simple modifications of the structure’s geometric parameters. The highly desired easy tuning property has led to the development of many plasmonic structures constructed using spheres [75, 76], ellipsoids [77], eggs [29], shells [78], circular disks [32], and rings [25] for various applications in bio- and chemical sensing [79, 80], designing plasmonic light sources and waveguides, and manipulating light at nanoscale. For bio- and chemical sensing applications, open quasi three-dimensional (disk and ring-like) structures are preferred over their closed counterparts because of their capacity to be in contact with greater
volumes of molecules within the near field of the plasmon modes [58].

Recently, generation of Fano resonances on nanostructures via interference of plasmon modes, an effect similar to electromagnetic induced transparency in atomic systems [18, 81], has become a topic of interest due to its promising applications in light manipulation [82], bio- and chemical sensing, and optical switching [15, 49]. Plasmonic Fano resonances are obtained from the coherent interference between plasmon modes; this can be achieved using either (anti-parallel) dipolar modes [22, 9] or a dipolar and a higher order mode (i.e., quadrapolar, octopolar modes) [14, 40, 83, 23, 84]. When the structure is electrically small and symmetric with respect to incident field’s polarization and/or direction of propagation, higher order modes cannot be excited by the incident field [26, 85, 39, 86]. One can increase the electrical size of structure (at the cost of ease of tunability) [25] or ‘break’ the structural symmetry [26] to permit the incident field’s energy to couple to the higher order modes. Symmetry breaking has been proven useful in excitation of higher order modes to generate plasmonic Fano resonances for various nanostructures constructed from shells [22, 83, 26], disks [32, 85] and rings [81, 39, 86]. Other examples of symmetry breaking methods include using conductive coupling between a theta-shaped ring rod and the wall of the ring enclosing it [43] and removing a wedge slice from a metallic nano-disk [44].

It is well known that any physical Fano resonance can be mathematically modeled using a multi-resonance coupled system of oscillator equations [26]. To this end, the mass spring model has been accurately applied in explanation of Fano resonances observed in the extinction cross-section (CS) spectrum of various nano-scale devices [26, 87, 88, 89]. The effect of double Fano resonance is studied in optical response of array of asymmetric pentamers using equivalent mass spring oscillator model [89].

In this chapter, the presence of two distinct Fano resonances in the optical response of a sub-wavelength planar metallic nanostructure to normally incident and linearly polarized electromagnetic field is demonstrated. The nanostructure is con-
Figure 2.1: Description of the incident electromagnetic field and the schematic views of the circular disk with (a) the concentric elongated cavity, (b) the shifted elongated cavity, and (c) the shifted and rotated elongated cavity.
structured from a circular gold disk embedding an elongated cavity. Schematic view of the structure and description of the incident electromagnetic field are given in Fig. 2.1(a). The higher order modes, which provide the mechanism for Fano resonance generation, are obtained via symmetry breaking. This is implemented by combining two approaches:

(i) The elongated cavity is shifted along the horizontal axis of the disk [Fig. 2.1(b)].

(ii) It is rotated around the normal of the disk [Fig. 2.1(c)].

Numerical simulations have demonstrated the presence of three distinct plasmon resonances in the extinction CS spectrum of this anti-symmetric geometry. Spectral tuning of these plasmonic resonances through modification of the geometry parameters produces two distinct Fano resonances in the visible spectrum. These results suggest that the disk with the shifted and rotated elongated cavity can be used as the building block of devices for generating slow light in bio- and chemical sensing applications. Additionally, in this chapter, the optical response of the proposed design is compared to the response of an RLC circuit, which is mathematically equivalent to that of a mass-spring oscillator.

It should be emphasized here the design of the circular gold disk embedding a shifted and rotated elongated cavity is distinguished from previously developed ring-like structures by two novel characteristics:

(i) Two distinct Fano resonances are generated in the extinction CS spectrum and this is achieved using only one layer of metal without the need for a metallic multi-layered shell. The fabrication of the proposed design is expected to be easier.

(ii) Elongated cavity is not cylindrically symmetric. This introduces the rotation angle of the cavity as another tuning variable and provides more flexibility for applications requiring operation in different frequency bands.
The remainder of the chapter is organized as follows. In Section 2.2.1, an initial design with a concentric elongated cavity is introduced and it is shown that this design supports a dipolar mode in the visible spectrum under a normally incident $x$-polarized plane wave. Note that the elongated cavity’s major axis is along the $x$-axis. In Section 2.2.2, it is shown that breaking the symmetry of the initial design with respect to the excitation by shifting the cavity along the $x$-axis permits higher order plasmon modes in the visible spectrum. The interference between the dipolar mode and the quadrupolar mode generates a Fano resonance dip in the spectrum. Additionally, tunability of the Fano resonance is also demonstrated: Decreasing the width of the cavity moves the locations of the dipolar and quadrupolar modes closer and improves the line shape of the Fano resonance. In Section 2.2.3, it is shown that the structural asymmetry introduced by rotating the shifted elongated cavity around the normal of the disk introduces another dipolar mode in the visible spectrum generating an additional Fano resonance dip. These Fano resonances can be tuned by modifying cavity’s rotation angle. In Section 2.3.1, it is shown that the total power drawn by an RLC circuit can be used to mathematically model the extinction CS of the proposed designs. Section 3.7 summarizes the contribution of this chapter and draws future research directions.

### 2.2 Design details and results

#### 2.2.1 Disk with concentric elongated cavity

To demonstrate the presence of a dipolar plasmonic mode in the visible spectrum, an initial design consisting of a gold disk and a concentric embedded elongated cavity is considered first [Fig. 2.1(a)]. The diameter and height of the disk and the length and width of the elongated cavity are $D = 100$ nm and $H = 10$ nm and $L = 65.5$ nm and $W = 35$ nm, respectively. The dimensions of the structure are chosen to induce
the Fano resonances in the visible and NIR range of the electromagnetic spectrum. It worth mentioning that as long as the overall size of the disk is a fraction of incident wavelength and scaling the geometry of the design (i.e., keeping the ratio of geometric lengths the same) does not significantly change the response of the system. For a detailed discussion on scaling optical response of a hole in a metal film see [90].

In the present study, we kept the overall size large enough to be able to induce the desired multimode optical response and also small enough to avoid large phase retardation effects, which would complicate the design of the structure. The structure is excited with a normally incident $x$- polarized plane wave. Due to the symmetry of the structure with respect to the excitation, only a dipolar mode is excited; higher order modes remain dark. This is clearly demonstrated by the extinction CS spectrum presented in Fig. 2.2. This dipolar mode is named $D_1$ in the remainder of the text. As shown by the surface charge distribution on the structure around $D_1$’s resonance frequency (inset of Fig. 2.2), $D_1$ possesses a non-zero dipole moment along the $x$-axis. Therefore the corresponding resonance in the extinction CS spectrum becomes visible under the excitation with an $x$-polarized incident field. However, higher order modes remain dark since they do not possess the dipole moment that would permit the incident field’s energy to couple to the modes.

It should be noted here that the plasmon hybridization theory [91] can be used to explain the plasmon mode interactions on rather complex nanostructures through hybridization of individual plasmon modes supported by the structure’s constitutive elements [91]. In this case, these constitutive elements are the circular disk and the elongated cavity embedded in an infinite uniform gold film. The plasmon hybridization theory models $D_1$ as a hybrid mode between the dipolar modes of the disk and the cavity. The surface charge distribution on the structure around $D_1$’s resonance frequency (inset of Fig. 2.2) demonstrates that the dipole moments of these individual dipolar modes are both in the $x$- direction making $D_1$ a bonding state hybrid mode.
Figure 2.2: Extinction CS spectrum of the circular disk with the concentric elongated cavity. The geometry parameters shown in Fig. 2.1(a) and the height of the structure are $D = 100$ nm, $L = 65.5$ nm, $W = 35$ nm, and $H = 10$ nm respectively. The inset shows the charge distribution on the structure at $762$ nm, marked with the blue dot on the plot. All the charges in the color plot are normalized between 1 and -1 (red and blue).

It should be noted here that the anti-boding state hybridized dipole mode cannot be excited with this incident field since the fully asymmetric charge distributions generated by the dipolar modes of the disk and the cavity cancels out the net dipole moment along the $x$-axis.

### 2.2.2 Disk with shifted elongated cavity

To allow for generation of higher order plasmon modes in the visible spectrum under the same excitation, a structural asymmetry is introduced in the initial design [Fig. 2.1(b)]. The elongated cavity with length $L = 65.5$ nm and width $W = 35$ nm is shifted along the $x$-axis by $O = 15.25$ nm. This breaks the structural symmetry (with respect to the excitation) of the initial design permitting incident field’s energy to couple to the higher order modes. This is clearly indicated by the extinction CS spectrum presented in Fig. 2.3(a); two distinct plasmon modes are identified: A dipolar mode (named $D_2$) and a quadrupolar mode (named $Q_1$).
Figure 2.3: (a) Extinction CS spectrum of the circular disk with the shifted elongated cavity. The geometry parameters shown in Fig. 2.1(b) and the height of the structure are $D = 100$ nm, $L = 65.5$ nm, $W = 35$ nm, $O = 15.25$ nm, and $H = 10$ nm respectively. The insets show the charge distributions on the structure at 656 nm (marked with the green dot on the plot), 696 nm (marked with the red dot), and 784 nm (marked with the blue dot). (b) Amplitude of the net dipole moment along the $x$-axis. (c) Extinction spectrum of the structure without the “wire”. The inset shows the charge distribution on the structure at 720 nm (marked with the blue dot on the plot).
Like $D_1$, $D_2$ is a bonding state hybrid mode between dipolar modes of the circular disk and the shifted elongated cavity embedded in an infinite uniform gold film (Section 2.2.1). This is clearly demonstrated by the charge distribution on the structure around $D_2$’s resonance frequency (inset of Fig. 2.3(a), frequency marked with the blue dot). The mode $Q_1$, which remains dark in the initial design, is a hybrid mode between the quadrupolar modes of the disk and the cavity. This is clearly shown by the charge distribution on the structure around $Q_1$’s resonance frequency (inset of Fig. 2.3(a), frequency marked with the green dot); the charge is distributed in the form of hybrid quadrupolar modes (one around the outer surface of the disk and another on the inner surface of the cavity). It should also be noted here that $Q_1$ is made active through symmetry breaking; its charge distribution has a non-zero net dipole moment along the $x$-axis. This clearly explains why the $x$-polarized incident field excites $Q_1$.

The asymmetric/non-concentric configuration of the circular disk and the elongated cavity creates a thin “wire” on the narrower side between the disk and the cavity. The plasmon modes’ electric field amplitudes reach to the maximum around the thinnest section of the wire indicating that the coupling between the modes is strongest along the thinnest section [92]. As a result, one can argue that the thickness of the wire determines the strength of plasmon coupling between modes of the disk and the cavity. Thinner wire means stronger hybridization and larger energy split between the bonding and anti-bonding states. It should be noted here that completely removing the wire (which results in a horseshoe shaped structure) eliminates $Q_1$. This is clearly shown by the extinction CS spectrum of the horseshoe shaped structure presented in Fig. 2.3(c). Obviously, even an asymmetric configuration for this shape fails to generate a higher order mode in the visible spectrum.

Extinction CS spectrum of the circular disk with the shifted elongated cavity [Fig. 2.3(a)] shows that $D_2$ and $Q_1$ overlap spectrally. The destructive interference
between these two modes generates a Fano resonance dip. The charge distribution around the dip (inset of Fig. 2.3(a) frequency marked with the red dot) reveals that the net dipole moment along the $x$-axis is cancelled due to overlapping of the modes $D_2$ and $Q_1$. This explains why the $x$-polarized incident field’s energy does not couple to the structure around the Fano resonance. The difference in the modes’ extinction CS amplitudes can be explained by the difference in the amount of energy they can receive from the incident field. The amount of energy coupled to a mode is related to the amplitude of that mode’s net dipole moment along the incident field’s polarization. This is demonstrated by Fig. 2.3(b), where the amplitude of the net dipole moment along the $x$-axis is provided; as expected, the locations of the peaks of the dipole moment and their relative amplitudes match to those of the extinction CS. Additionally, this figure clearly demonstrates the destructive cancellation of the dipole moment along the $x$-axis around the Fano resonance. Here, the term “cancellation” refers to the suppression of net dipole moment via opposite-sign contributions from charge distributions induced by each of the plasmon modes [inset in Fig. 2.3(b)].

Next, the effect of filling the shifted elongated cavity on the resonance frequencies of $D_2$ and $Q_1$ is characterized. The cavity is filled with silica (refractive index $n = 1.5$) and as expected due to change in the optical path length of the resonance and demonstrated by the extinction CS spectrum provided in Fig. 2.4(a) resonances of $D_2$ and $Q_1$ red shift [93]. Additionally, by filling the cavity with silica increases the effective electrical size of the cavity surface (medium wavelength in silica is smaller). This allows for larger room for quadrupolar modes charges to distribute on the cavity surface and results in greater changes in the dipole moment along the direction incident fields polarization. Increase in the electrical size of the cavity has a less significant effect on the dipolar modes dipole moment since the charge has a much simpler distribution (positive and negative peak charges are on opposite symmetry axis). Overall, the quadrupolar modes characteristics are more sensitive to refractive
Figure 2.4: Tunability of the design with the circular disk and the shifted elongated cavity. (a) Extinction CS spectrum of the design with the cavity filled with silica (refractive index $n = 1.5$). (b) Extinction CS spectra of the designs where the cavity’s width is changed from $W = 20$ nm to $W = 45$ nm with a step of 5 nm while the other parameters are $D = 100$ nm, $L = 65.5$ nm, $O = 15.25$ nm, and $H = 10$ nm.
index of the material filling in the cavity. This also suggests that the electrical size of the cavity can be used to tune the Fano resonance. To further demonstrate this, cavity’s width is changed from \( W = 20 \text{ nm} \) to \( W = 45 \text{ nm} \) with a step of 5 nm. Fig. 2.4(b) plots the extinction CS spectrum for each value of \( W \); the resonances of the \( D_2 \) and \( Q_1 \) red shift as the width of the cavity increases. Additionally, the figure reveals that the overlap between \( D_2 \) and \( Q_1 \) increases as the width of the cavity decreases (since the spectral shift in the resonance of \( D_2 \) is larger than that of \( Q_1 \)). Consequently, the asymmetric line shape of the Fano resonance improves with the decreasing cavity size (i.e., fill factor).

2.2.3 Disk with shifted and rotated elongated cavity

Rotating the shifted elongated cavity around the normal of the disk introduces an additional structural asymmetry to the design [Fig. 2.1(c)]. Here, \( \theta \) is the angle that the elongated cavity’s major axis makes with the \( x \)-axis at its center. Consider, for example, the design with \( \theta = 40^\circ \); an \( x \)-polarized plane wave normally incident on this structure generates three plasmon modes as demonstrated by the extinction CS spectrum provided in Fig. 2.5(a). Two of these modes are dipolar modes (named \( D_3 \) and \( D_4 \)) and one of them is a quadrupolar mode (named \( Q_2 \)).

As with the previously described modes, the plasmon hybridization theory can be used to describe the physical properties of \( D_3 \), \( D_4 \), and \( Q_2 \). Like \( D_1 \) (Section 2.2.1) and \( D_2 \) (Section 2.2.2), \( D_3 \) and \( D_4 \) are hybrid modes between the dipolar modes of the circular disk and the shifted and rotated elongated cavity embedded in an infinite uniform gold film. This is clearly demonstrated by the charge distributions on the structure around the resonance frequencies of \( D_3 \) and \( D_4 \) (inset of Fig. 2.5(a), frequencies marked with the blue and black dots, respectively). Dipole of moment of \( D_3 \)’s charge distribution is largest along the major axis of the cavity but still has a non-zero value along the \( x \)-axis and the dipole moment of \( D_4 \)’s charge distribution...
Figure 2.5: (a) Extinction CS spectrum of the circular disk with the shifted and rotated elongated cavity. The geometry parameters shown in Fig. 2.1(c) and the height of the structure are $D = 100 \text{nm}$, $L = 65.5 \text{nm}$, $W = 35 \text{nm}$, $O = 15.25 \text{nm}$, $\theta = 40^\circ$, and $H = 10 \text{nm}$, respectively. The insets show the charge distribution on the structure at 622 nm (marked with the green dot on the plot), 674 nm (marked with the red dot), 788 nm (marked with the blue dot), 904 nm (marked with the cyan dot), and 1020 nm (marked with the black dot) (b) Amplitude of the net dipole moment along the $x$-axis.
is largest along the $x$-axis. Like $Q_1$ (Section 2.2.2), $Q_2$ is a hybrid mode between the quadrupolar modes of the disk and the cavity. Charge distribution on the structure around $Q_2$’s resonance frequency (inset of Fig. 2.5(a), frequency marked with the green dot) shows that $Q_2$ also has a non-zero dipole moment along the $x$-axis. Presence of non-zero dipole moments along the $x$-axis for $D_3$, $D_4$, and $Q_2$ explains why the $x$-polarized incident field excites these modes.

As clearly shown in Fig. 2.5(a) mode $D_3$ spectrally overlaps with both $D_4$ and $Q_2$. The destructive interference between $Q_2$ and $D_3$ and $D_3$ and $D_4$ generate two Fano resonance dips in the visible spectrum. The presence of destructive interference between $Q_2$ and $D_3$ and $D_3$ and $D_4$ is demonstrated by the charge distributions around the Fano resonance dips (the inset of Fig. 2.5(a) frequencies marked with the red and cyan dots). Around the Fano resonance frequencies, the net dipole moment along the $x$-axis is cancelled due to spectral overlapping of the modes, which generate dipole moments in opposite directions. This explains why the $x$-polarized incident fields energy does not couple to the structure around the Fano resonances.

As discussed in Section 2.2.2 the extinction CS amplitude of a mode depends on the energy it can receive from the incident field and hence the net dipole moment along the field’s polarization. This is demonstrated by Fig. 2.5(b) where the amplitude of the net dipole moment along the $x$-direction is provided; as expected, the locations of the peaks of the dipole moment and their relative amplitudes match to those of the extinction CS.

Next, the effect of the rotation angle $\theta$ [measured from the $x$-axis, Fig. 2.1(c)] of the shifted elongated cavity on the resonance frequencies of $D_3$, $D_4$, and $Q_2$ is characterized: $\theta$ is changed from $10^\circ$ to $90^\circ$ with a step of $20^\circ$; the extinction CS spectrum computed for each value of $\theta$ is provided in Fig. 2.6. As demonstrated by the figure, the extinction CS amplitude peak that corresponds to $D_4$ gets intensified while those that correspond to $D_3$ and $Q_2$ turn off as $\theta$ changes from $10^\circ$ to $90^\circ$. 
Figure 2.6: Tunability of the design with the circular disk and the shifted and rotated elongated cavity. Extinction spectra of the designs where the cavity’s rotation angle is changed 10° to 90° with a step of 20° while the other parameters are $D = 100\,\text{nm}$, $L = 65.5\,\text{nm}$, $O = 15.25\,\text{nm}$, and $H = 10\,\text{nm}$. 
Figure 2.7: Comparison between the rotation of cavity and disk around their respective centers for $\theta = 90^\circ$.

As discussed before, this can be explained by the change in the mode’s net dipole moment along the $x$-axis as $\theta$ changes. For example, for $\theta = 90^\circ$, $D_3$’s dipole moment along $x$-axis vanishes, and the mode cannot be excited with an $x$-polarized incident field any more. As a result the extinction CS amplitude of $D_3$ vanishes.

Finally, the responses of the disk with the shifted and rotated elongated cavity and the rotated disk with the shifted elongated cavity are compared and shown by Fig. 2.7. Both the rotations are $90^\circ$. As expected the responses are similar since the position of the cavity is slightly different in these cases. The resonance frequency of the dipolar mode $D_4$ is slightly blue-shifted for the disk with the shifted and rotated elongated cavity.

2.3 Methods

2.3.1 RLC circuit model

The optical response of the shifted (and rotated) elongated cavity can be replicated using an electrical oscillator that can support multiple resonances [88]. A RLC circuit
Figure 2.8: (a) Description of the RLC circuit that supports three resonances. (b) Normalized spectra of $P$ for the circuit with $\gamma_1 = 21.76$ THz, $\gamma_2 = 23.03$ THz, $\omega_1 = 446.98$ THz, $\omega_2 = 397.19$ THz, $\Omega_{12} = 168.50$ THz, and $\Omega_{13} = \Omega_{23} = 0$, and the extinction CS for the design with $D = 100$ nm, $W = 35$ nm, $L = 65.5$ nm, $O = 15.25$ nm, and $H = 10$ nm. (c) Normalized spectra of $P$ for the circuit with $\gamma_1 = 27.32$ THz, $\gamma_2 = 25.52$ THz, $\gamma_3 = 18.23$ THz, $\omega_1 = 464.29$ THz, $\omega_2 = 382.14$ THz, $\omega_3 = 321.49$ THz, $\Omega_{12} = 188.34$ THz, $\Omega_{13} = 125.77$ THz, and $\Omega_{23} = 145.20$ THz, and the extinction CS for the design with $D = 100$ nm, $W = 35$ nm, $L = 65.5$ nm, $O = 15.25$ nm, $H = 10$ nm, and $\theta = 40^\circ$. 
shown in Fig. 2.8(a) is used for this purpose. The spectrum of the power drawn by this RLC circuit can be used to mathematically imitate the extinction CS spectrum of the designs with two plasmon modes $D_2$ and $Q_1$ (Section 2.2.2) and three plasmon modes $D_3$, $D_4$, and $Q_2$ (Section 2.2.3). The circuit consists of three loops of resistive, inductive, and capacitive elements ($R_i$, $L_i$, and $C_i$, $i = 1, 2, 3$), which are coupled using capacitive elements ($C_{12}$, $C_{13}$, and $C_{23}$). Each loop corresponds to one plasmon mode: Combination of inductive and capacitive elements in each loop generates a resonance while the resistive element accounts for the energy dissipation (due to radiation and ohmic loss). The electromagnetic field incident on the designs is modeled as a time harmonic voltage source, $V_s(t) = \Re\{V e^{j\omega t}\}$, feeding the loop 2, which represents the dipolar mode that is excited by the incident field. Applying Kirchhoff voltage law to each of the loops in the direction of the arrows as shown in Fig. 2.8(a) yields a coupled system of equations

$$
\begin{align*}
-\omega^2 L_1 + j\omega R_1 + \frac{1}{C_1} + \frac{1}{C_{12}} + \frac{1}{C_{13}} I_1 - \frac{I_2}{C_{12}} - \frac{I_3}{C_{13}} &= 0 \\
-\omega^2 L_2 + j\omega R_2 + \frac{1}{C_2} + \frac{1}{C_{12}} + \frac{1}{C_{23}} I_2 - \frac{I_1}{C_{12}} - \frac{I_3}{C_{23}} &= V/L_2 \quad (2.1) \\
-\omega^2 L_3 + j\omega R_3 + \frac{1}{C_3} + \frac{1}{C_{13}} + \frac{1}{C_{23}} I_3 - \frac{I_1}{C_{13}} - \frac{I_2}{C_{23}} &= 0
\end{align*}
$$

where $I_i$ represents the current on loop $i$, $i = 1, 2, 3$. Expressing $I_i$ as the rate of change of charge, i.e., $I_i = j\omega q_i$, in the coupled system of equations (2.1), one can obtain:

$$
\begin{align*}
\Gamma_1 q_1 - \Omega_{12}^2 q_2 - \Omega_{13}^2 q_3 &= 0 \\
\Gamma_2 q_2 - \Omega_{12}^2 q_1 - \Omega_{23}^2 q_3 &= V/L_2 \\
\Gamma_3 q_3 - \Omega_{13}^2 q_1 - \Omega_{23}^2 q_2 &= 0 \quad (2.2)
\end{align*}
$$

where $\Gamma_i = -\omega^2 + j\omega\gamma_i + \omega_i^2$, $\omega_i = 1/((L_i C_{eqi})^{0.5}$ is the natural resonance frequency
of the loop $i$, $\gamma_i = R_i/L_i$ and $C_{eqi}$ represent its damping coefficient and equivalent capacitance (assuming other loops are open), respectively, and $\Omega_{ij} = 1/(L_iC_{ij})^{0.5}$ is the coupling coefficient between the loops $i$ and $j$. Here, $C_{eqi}$, $i = 1, 2, 3$, are given by $1/C_{eq1} = 1/C_1 + 1/C_{12} + 1/C_{13}$, $1/C_{eq2} = 1/C_2 + 1/C_{12} + 1/C_{23}$, and $1/C_{eq3} = 1/C_3 + 1/C_{13} + 1/C_{13}$.

Given the phasor of the voltage source, $V$, to obtain an expression for the time average total power drawn by the circuit, $P$, one should known $I_2$. Coupled system of equations (2.2) can be solved for $q_2$; then an exion for $I_2$ can be obtained using $I_2 = j\omega q_2$. Inserting this in $P = 0.5\mathrm{Re}\{V I_2^*\}$ yields an expression for $P$:

\[
P = 0.5|V|^2\mathrm{Re}\left\{j\omega \left(\Omega_{13}^4 - \Gamma_1 \Gamma_3\right) / \left( L_2 \left[ 2\Omega_{12}^2 \Omega_{13}^2 \Omega_{23}^2 + \Omega_{23}^4 \Gamma_1 + \Omega_{12}^4 \Gamma_3 + \Gamma_2 \left( \Omega_{13}^4 - \Gamma_1 \Gamma_3 \right) \right] \right) \right\}
\]

As mentioned above, $P$ can be used to mathematically imitate the extinction CS of the designs supporting $D_2$ and $Q_1$ and $D_3$, $D_4$, and $Q_2$. The curve described by equation (2.3) is numerically fitted to the extinction CS curves obtained via finite element method using the Levenberg-Marquardt algorithm implement within OriginLab commercial software [94]. The algorithm produces the parameters in equation (2.3), which are then used to find the values of the inductances, capacitances, and resistances in the circuit. First, the design that supports $D_2$ and $Q_1$ is considered. For this case, $\Omega_{13} = \Omega_{23} = 0$, since loops 2 and 1 model $D_2$ and $Q_1$, respectively, while loop 3 is left unpowered, i.e., short-circuited. As shown in Fig. 2.8(b), choosing $\gamma_1 = 21.76$ THz, $\gamma_2 = 23.03$ THz, $\omega_1 = 446.98$ THz, $\omega_2 = 397.19$ THz, and $\Omega_{12} = 168.50$ THz, normalized spectrum of $P$ is matched to that of the extinction CS for the design with $D = 100$ nm, $W = 35$ nm, $L = 65.5$ nm, $O = 15.25$ nm, and $H = 10$ nm. Next, the design that supports $D_3$, $D_4$, and $Q_2$ is considered. For this case, loops 1, 2, and 3 are all active and they model $D_3$, $D_4$, and $Q_2$, respectively. As shown in Fig. 2.8(c), choosing
\( \gamma_1 = 27.32 \text{ THz}, \gamma_2 = 25.52 \text{ THz}, \gamma_3 = 18.23 \text{ THz}, \omega_1 = 464.29 \text{ THz}, \omega_2 = 382.14 \text{ THz}, \omega_3 = 321.49 \text{ THz}, \Omega_{12} = 188.34 \text{ THz}, \Omega_{13} = 125.77 \text{ THz}, \) and \( \Omega_{23} = 145.20 \text{ THz}, \) normalized spectrum of \( P \) is matched to that of the extinction CS for the design with \( D = 100 \text{ nm}, W = 35 \text{ nm}, L = 65.5 \text{ nm}, O = 15.25 \text{ nm}, H = 10 \text{ nm}, \) and \( \theta = 40^\circ. \)

It should be noted here that damping coefficients \( \gamma_i \) have similar values for all three modes indicating that these modes have similar radiation and absorption characteristics. But this does not prevent these modes from destructively interfering with each other and permit the generation of Fano resonance/PIT. The resonance frequencies \( \omega_i \) are clearly close enough for the modes to have overlapping frequencies.

### 2.3.2 Simulation parameters

The electromagnetic wave interactions on the plasmonic nanostructure design proposed here cannot be computed using (semi-) analytical methods. To this end, all field interaction computations are carried out using the RF module of the commercially available Finite Element based software package COMSOL Multiphysics 3.5a [95]. The computation domain is truncated using a 50 nm thick perfectly matched layer (PML) introduced on a spherical surface with radius 250 nm (measured from the center of the disk). On the outer surface of the PML, scattering boundary conditions are enforced. The scattered field formulation is used to introduce the normally incident \( x \)-polarized plane wave into the computation domain.

The empirically determined dispersive and complex refractive index of the bulk gold, which is known as Johnson and Christy model [96], is used in all COMSOL simulations. A table listing values of the complex dielectric constant measured at frequency samples are provided in [96]; linear interpolation is used to compute dielectric constant values at frequencies in between these samples.

The absorption CS is calculated by integrating the time average resistive heating in the volume of the gold disk [20]. The scattering CS is calculated by integrating
the time average radiated field power density on a spherical surface, which encloses the structure, in the far-field region. The extinction CS is obtained by summing the absorption and scattering CSs.

The charges induced on the surface of the structure are computed from the boundary conditions on the normal component of the electric field. The charges induced in the volume of the structure are computed from the divergence of the electric field. In dipole moment computations, both surface and volume charges are taken into account.

2.4 Discussion and possible limitations

Results presented in this chapter suggest that the proposed design, which involves a planar and circular disk embedding a shifted and rotated elongated cavity, can be used as the building block of devices for generating slow light in bio- and chemical sensing applications. However, two limitations that might hinder the potential use of the proposed design in these applications are lack of dynamic tunability and polarization dependence of the output. These limitations can be overcome by modifying the design via hybridization with graphene as described in the next chapter.

2.5 Summary

The presence of Fano resonances in the optical response of a sub-wavelength planar metallic nanostructure to normally incident and linearly polarized electromagnetic field is demonstrated. The nanostructure is constructed from a circular gold disk embedding an elongated cavity. The symmetry of the structure with respect to the incident field is broken by shifting and rotating the elongated cavity. The spectral overlaps between the dipolar plasmon mode and the higher order ones, which are induced due to symmetry breaking, result in two distinct Fano resonances in the
visible spectrum. It is shown that these resonances can be tuned by varying the geometry parameters, especially the width and the rotation angle of the elongated cavity. Additionally, extinction CS of the proposed design is compared to the total power drawn by an RLC circuit, representing a mathematical model analogue to a mass-spring oscillator.
Chapter 3

A dynamically tunable Fano resonator

3.1 Introduction

Symmetry breaking is often used to design multiple Fano resonances. In the previous chapter a tunable through (through geometry) Fano-resonator has been described using symmetry breaking. For example the excitation of the higher order SPPs is often made possible by means of symmetry breaking [15, 20, 24]. However, it also leads to polarization dependence of the resonator response. A symmetric design capable of polarization independent response of Fano resonance is often desired. Additionally, the material response of plasmonic materials e.g. gold, silver are static by their nature. Therefore, to achieve dynamic tunability new plasmonic materials are required to build Fano resonators. This chapter addresses these issues to design a dynamically tunable Fano resonator using tunable ultra-thin graphene material integrated with gold structure.

Generation of physical phenomena equivalent to EIT at terahertz (THz) frequencies is also currently one of the most exciting topics of plasmonics research [45]. Since most of the biomolecules have their vibrational modes oscillating at THz frequencies [37, 97], this means that EIT generated at these frequencies offers a viable way for
biosensing. The drastic “slowing” of light around the narrow Fano resonance results in an increased sensitivity to changes in the medium’s refractive index. Plasmonic EIT could also be used in designing efficient switches for modulating the amplitude and phase of waves transmitted through metamaterials [98]. Possibility of designing ultra-sensitive bio-detectors and efficient switches urges the investigation of plasmonic metamaterials capable of supporting Fano resonances at THz frequencies. The unique and highly tunable electrical properties of graphene [99] observed within this band of the spectrum render it an attractive candidate as a building block of such metamaterials.

Since its first practical isolation by Novoselov and Geim in 2004 [99], graphene solicited a keen interest among physicists and engineers. This could be attributed to graphene’s unprecedented properties that cannot be found in any other material [100]. High electron mobility [101], significant white light absorption [102, 103, 98], ability to support SPPs [104, 105, 106, 107] are among these characteristics that are relevant in the fields of electromagnetics, optics, and photonics [108].

In this chapter, graphene’s ability to support SPPs at THz frequencies is exploited to design a Fano resonator that hybridizes SPPs generated on graphene and gold surfaces. Graphene surface plasmon polaritons (GSPPs) have several advantages when compared to SPPs generated on metallic surfaces: GSPPs have higher volume confinement (exceeding $10^6$ times the diffraction limit), are easier to tune (obtained via applying a gate voltage to the graphene), and propagate longer distances and have narrower spectral support (due to the lower intrinsic losses in graphene) [109, 110]. Not surprisingly, these superior features of GSPPs have fueled research in several directions such as development of GSPP waveguides [111, 112], THz antennas [113, 114, 115], perfect absorbers [62, 64], novel Fourier optics devices [116], THz cloaks [117, 118], photonic crystal nano-cavities [119], modulators [120] and sensors [121].

The hybrid graphene-gold Fano resonator proposed in this chapter is a doubly
periodic array of a unit cell constructed using a square graphene patch located at the center of a square gold frame. The Fano resonance is obtained from the destructive interference between the dipolar SPPs generated on the graphene patch and the gold frame at THz frequencies and its spectral shape and location can easily be tuned by applying a gate voltage to the graphene patch.

3.2 Design details and results

3.2.1 Physical mechanism

The Fano resonator proposed in this chapter is a doubly periodic array of a unit cell that consists of a square graphene patch located at the center of a square gold frame. The resonator is embedded in a dielectric substrate. [see Fig. 3.1]. The proposed Fano resonator is excited with a plane wave propagating in the $z$-direction with electric field polarized in the $x$-direction [Figs. 3.1(b) and 3.1(c)]. It should be noted here that due to the symmetry of the unit cell and the same periodicity in $x$- and $y$- directions, the response of the resonator is polarization independent. When excited with this incident field separately, the gold frame and the graphene patch support dipolar SPPs. As a result, the resonator constructed using the gold frame and the graphene patch supports an SPP mode hybridized between these two dipolar modes. Since the dipolar SPP induced on the frame has a much broader spectral support than the one induced on the graphene patch due to the presence of higher intrinsic losses in gold, these two modes’ destructive interference generates a Fano line-shape in the response of the resonator. It should be noted here that the plasma frequencies of gold and graphene are separated by a large offset. This means that the resonance frequencies corresponding to the dipolar SPPs induced on the gold frame and the graphene patch are expected to be separated by a large gap. To move the resonance frequencies closer to each other and have the SPPs’ spectral supports
overlap at THz frequencies, the geometrical dimensions of the frame and the patch are chosen to be in µm scale as shown in Fig. 3.1(a).

Obviously, in this design, SPP of the graphene patch acts like the “dark mode” of the traditional Fano resonator designs made of only metals [15]. Additionally, unlike these traditional resonators, the proposed design does not require its symmetry to be “broken” since the narrower mode can be directly excited by the incident field even if the structure is fully symmetric. The spectral location and line-shape of the graphene’s narrow dipolar SPP is determined by graphene’s complex relative permittivity \( \varepsilon_{V,G} \), which can be controlled by adjusting the chemical potential \( \mu_c \) (see Methods Section on Material Models for details). Variation in \( \mu_c \) can be achieved by applying a gate voltage to the graphene patch using nearly transparent electrodes without perturbing the response of the resonator as suggested recently in reference [98].

### 3.2.2 Proof of concept via numerical experiments

The hybridization of the dipolar SPPs induced on the gold frame and the graphene patch is demonstrated by an example. For this simulation, the dimension of the gold frame \( S_1 = 5.5 \, \mu m \), the dimension of the graphene patch \( S_2 = 1.6 \, \mu m \), the relative dielectric permittivity of the substrate \( \varepsilon_d = 3.5 \), and graphene’s electron mobility \( \mu = 10,000 \, cm^2/Vs \) and chemical potential \( \mu_c = 1500 \, meV \). It should be noted here that the value assigned to \( \mu \) is a rather conservative choice considering the latest experimental results [108]. The transmittance of three structures constructed using unit cells with only the gold frame, only the graphene patch, and both the gold frame and the graphene patch are computed [Figs. 3.2(a), 3.2(b), and 3.2(c), respectively]. As expected, the dipolar SPPs induced on the gold frame (marked as \( D_1 \)) and the graphene patch (marked as \( D_2 \)) have broad (continuum-like) and very narrow spectral supports, respectively. Figure 3.2(c) clearly demonstrates the
Figure 3.1: (a) Top view of the unit cell with dimensions. (b) Cross section view and the normally incident excitation. (c) Doubly periodic array of the unit cell and the normally incident excitation.
Figure 3.2: (a) Transmittance of only the gold frame. $S_1 = 5.5 \, \mu m$ and $\varepsilon_d = 3.5$. SPP is marked as $D_1$. (b) Transmittance of only the graphene patch for different values of $\mu_c$. $S_2 = 1.6 \, \mu m$, $\mu = 10,000 \, cm^2/Vs$, and $\varepsilon_d = 3.5$. SPP is marked as SPP $D_2$. Transmittance of the resonator with both the gold frame and the graphene patch. $S_1 = 5.5 \, \mu m$, $S_2 = 1.6 \, \mu m$, $\varepsilon_d = 3.5$, $\mu = 10,000 \, cm^2/Vs$, and $\mu_c = 1500 \, meV$. (c) Amplitude and (d) phase.
asymmetric Fano-like spectral line-shape and a narrow EIT window in the response of the resonator constructed using both the gold frame and the graphene patch, which results from destructive interference of $D_1$ and $D_2$.

The dipolar nature of the SPPs is exhibited in Fig. 3.3 showing the surface charge distributions and the magnetic field norm computed at several frequency points. Fields due to $D_1$ are clearly more dominant at point I, which is far away from the resonance frequency of $D_2$. Surface charge distributions at the frequency points II, III, and IV (around the Fano resonance), clearly demonstrate that $D_2$ interferes with $D_1$. Additionally, comparison of charge distributions (and magnetic field norms) at points II and III reveals that the sharp roll-off of the transmittance between the EIT point at 8.35 THz and the graphene’s dipolar SPP at 9 THz is due to the phase change of the field distribution at the points II and III.

The effect of geometrical dimensions on the response of the Fano resonator is characterized next. For the first set of simulations, $S_1 = 5.5 \, \mu m$, $\varepsilon_d = 3.5$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500 \, \text{meV}$, while $S_2$ is varied between 1 $\mu m$ and 2 $\mu m$. Transmittance of the resonator is computed for each value of $S_2$ [Fig. 3.4(a)]. Increasing $S_2$ (for example by setting it to 2 $\mu m$) red-shifts the resonance of $D_2$ as it increases the graphene patch’s effective dipole length. This moves the resonant frequencies of $D_1$ and $D_2$ closer to each other and forces them to couple more strongly. As a result, a higher increase in the transmittance within the EIT band [with respect to the transmittance of only $D_1$ plotted in Fig. 3.4(a) as thin blue line] is observed. On the other hand, when $S_2$ is decreased (for example by setting it to 1 $\mu m$), the resonance frequencies of $D_1$ and $D_2$ get sufficiently detuned. In this case, transmittance follows very closely the transmittance of only $D_1$ with a much smaller relative increase in the EIT band. For the second set of simulations, $S_2 = 1.6 \, \mu m$, $\varepsilon_d = 3.5$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500 \, \text{meV}$, while $S_1$ is varied between 4 $\mu m$ and 6 $\mu m$. Transmittance of the resonator is computed for each value of $S_1$ [Fig. 3.4(b)]. As expected, increasing $S_1$
Figure 3.3: (a) Surface charge distributions on the unit cell computed at frequency points I, II, III, and IV corresponding to the frequencies: 5.3, 7.7, 8.35 and 9 THz. $S_1 = 5.5\, \mu\text{m}$, $S_2 = 1.6\, \mu\text{m}$, $\varepsilon_d = 3.5$, $\mu = 10,000\, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500\, \text{meV}$. The color scale for the positive and negative surface charges are normalized between (-1 and 1). (b) Same as in (a) but for the distribution of the norm of the magnetic field in the plane of the unit cell x-y.
red-shifts the resonance of $D_1$ as it increases the frame’s effective dipole length. For $S_1 = 6 \, \mu m$, a higher increase in the transmittance within the EIT band [with respect to the transmittance of only $D_1$ plotted in Fig. 3.4(b) as thin blue line] is observed. For $S_1$ between 4.5 $\mu m$ and 4 $\mu m$, the asymmetric Fano line-shape appears on the left side of the resonance frequency of $D_1$. These results clearly indicate that depending on the target application, the dimensions of the graphene patch and the gold frame can be fine-tuned. For example, if one wants to design an optical modulator using the Fano resonator proposed here, a greater modulation depth can be achieved by choosing the geometry dimensions that result in a large variation in the transmittance within the EIT band.

The effect of graphene’s intrinsic loss, i.e., the value of its electron mobility, $\mu$, on the response of the Fano resonator is also analyzed. For this set of simulations, $S_1 = 5.5 \, \mu m$, $S_2 = 1.6 \, \mu m$, $\varepsilon_d = 3.5$, and $\mu_c = 1500$ meV, while $\mu$ is swept from 1,000 cm$^2$/Vs to 250,000 cm$^2$/Vs. Figure 3.4(c) shows the transmittance of the resonator computed for each value of $\mu$. For lower values of $\mu$, i.e., for higher loss, the absorption channel becomes dominant and the transmission efficiency is deteriorated as expected. For realistic values of $\mu$ around 10,000 cm$^2$/Vs, the response of the Fano resonator is good; the transmittance efficiency reaches almost 60%.

Finally, the effect of the substrate on the response of the resonator is characterized. For this set of simulations, $S_1 = 5.5 \, \mu m$, $S_2 = 1.6 \, \mu m$, $\mu = 10,000$ cm$^2$/Vs, and $\mu_c = 1500$ meV, while $\varepsilon_d$ is varied between 1 (no substrate) and 5. The transmittance of the resonator is computed for each value of $\varepsilon_d$ [Fig. 3.4(d)]. It is clearly shown in the figure that a gradual red-shift is observed in the response of the resonator as $\varepsilon_d$ is increased. A gradual decrease in the maximum amplitude in transmittance is observed with an increase in $\varepsilon_d$. 
Figure 3.4: (a) Transmittance of the resonator with $S_1 = 5.5 \mu\text{m}$, $\varepsilon_d = 3.5$, $\mu = 10,000 \text{ cm}^2/\text{Vs}$, and $\mu_c = 1500 \text{ meV}$ for various values of $S_2$. The transmittance of only the gold frame with $S_1 = 5.5 \mu\text{m}$ is plotted as a reference in thin blue line. (b) Transmittance of the resonator with $S_2 = 1.6 \mu\text{m}$, $\varepsilon_d = 3.5$, $\mu = 10,000 \text{ cm}^2/\text{Vs}$, and $\mu_c = 1500 \text{ meV}$ for various values of $S_1$. The transmittance of only the gold frame with $S_1 = 6 \mu\text{m}$ is plotted as a reference in thin blue line. (c) Transmittance of the resonator with $S_1 = 5.5 \mu\text{m}$, $S_2 = 1.6 \mu\text{m}$, $\varepsilon_d = 3.5$, and $\mu_c = 1500 \text{ meV}$ for various values of $\mu$. (d) Transmittance of the resonator with $S_1 = 5.5 \mu\text{m}$, $S_2 = 1.6 \mu\text{m}$, $\varepsilon_d = 3.5$, and $\mu_c = 1500 \text{ meV}$ for various values of $\varepsilon_d$. 
3.3 Applications

*Switching:* The EIT window generated via the destructive interference of the dipolar SPPs induced on the gold frame and the graphene patch is tuned by controlling a gate voltage applied to the graphene patch (as discussed for example in recent studies [98]). To simulate the effect of the variation in the gate voltage, graphene’s chemical potential $\mu_c$ is swept between 500 meV and 1500 meV while $\varepsilon_d = 3.5$ and $\mu = 10,000 \text{ cm}^2/\text{Vs}$.

The transmittance of the structure constructed using unit cells with only the graphene patch with $S_2 = 1.6 \mu\text{m}$ is computed for various values of $\mu_c$ [Fig. 3.2(b)]. The figure clearly demonstrates that increasing $\mu_c$ leads to a blue shift in the resonance frequency of $D_2$ and comparatively stronger extinction amplitude $1 - T$ (where $T$ denotes the transmittance) at the resonance frequency.

Similarly, the amplitude and phase of the transmittance of the structure constructed using unit cells with the gold frame with $S_1 = 5.5 \mu\text{m}$ and the graphene patch with $S_2 = 1.6 \mu\text{m}$ is computed for the same values of $\mu_c$ [Figs. 3.5(a) and 3.5(b)]. The figures clearly show that the spectral location and the shape of the EIT window can be tuned by varying $\mu_c$. This easily tunable EIT window can be utilized as a mechanism to make switches at THz frequencies. For example, as shown in Fig. 3.6(a), the transmittance at 7.94 THz can be switched between 0.4% to 53% by simply varying the chemical potential $\mu_c$ by an amount of $\Delta \mu_c = (1430 - 1280) \text{ meV} = 150 \text{ meV}$. As a result a maximum modulation index of 0.52 is achieved through a small variation of $\Delta \mu_c = 150 \text{ meV}$. The voltage-controlled resonator has in addition the potential to be used as a phase modulation device. The highly dispersive propagation within the EIT band have a steep spectral variation in transmission phase $\phi$ [Fig. 3.2(c)]. This feature allows to modulate the phase of the transmitted signal to a substantial degree. As shown in Fig. 3.6(b), the phase of the transmission at 8.22 THz can be changed by $\Delta \phi = 0.68 \text{ rad}$, by simply varying the chemical potential $\mu_c$ by the same amount.
Figure 3.5: (a) Transmittance of the resonator with $S_1 = 5.5 \, \mu m$, $S_2 = 1.6 \, \mu m$, $\varepsilon_d = 3.5$, and $\mu = 10,000 \, \text{cm}^2/\text{Vs}$ for various values of $\mu_c$ between 500 meV and 1500 meV. (b) Same as in (a) but for the phase of the transmission. The dashed white lines highlight the plasmonic EIT-like zone.
as for the amplitude. The amplitude and phase modulation index can be further improved by optimization of spectral positions for the interference of the resonances. For example, maximum modulation index for the amplitude can be increased to 0.65 by setting $S_1 = 6 \mu m$ [Fig. 3.4(b)]. The commercial applications for this integrated THz modulator are in the areas of communication systems, high speed Mach-Zehnder modulators, phase array antennas and time-domain spectroscopy [122].

**Slow Light and Sensing:** The effective refractive and group indices, $n_e$ and $n_g$, of the resonator design with $S_1 = 5.5 \mu m$, $S_2 = 1.6 \mu m$, $\varepsilon_d = 3.5$, $\mu = 10,000$ cm$^2$/Vs, and $\mu_c = 1500$ meV are extracted. To this end, a homogenous slab with refractive index $n_e$, which generates the same S-parameters as the proposed design, is found using the retrieval method described in reference [123]. Then, the effective group index is computed using the relation:

$$n_g(\omega) = n_e(\omega) + \omega \frac{\partial n_e(\omega)}{\partial \omega}$$

The retrieved $n_e$ and $n_g$ are shown in Figs. 3.7(a) and 3.7(b), respectively; the value of $n_g$ exceeds 1,400 within the EIT window. This value is much higher than that of the other plasmonic resonators solely made of metals [45]. High values of $n_g$ clearly demonstrate that the proposed Fano resonator design has the potential to be used in slow light applications including ultra-sensitive biomolecule detection.

### 3.4 Material models

The complex dielectric constant of gold is accurately modeled at THz frequencies using the Drude model with plasma frequency $\omega_p = 1.37 \times 10^{16}$ rad/s and damping constant $\gamma_c = 39.47 \times 10^{12}$ rad/s [124]. The complex surface conductivity $\sigma_{S,G}$ for a graphene layer is calculated from Kubo’s formula [98, 104]:

$$\sigma_{S,G}(\omega) = \sigma_{\text{intra}}(\omega) + \sigma_{\text{inter}}(\omega).$$  \hspace{1cm} (3.1)
Figure 3.6: Switching applications: (a) Transmittance as function of $\mu_c$ for different values of the operation frequency: 7.1, 7.7, 7.94 and 8.22 THz. $S_1 = 5.5 \, \mu m$, $S_2 = 1.6 \, \mu m$, $\varepsilon_d = 3.5$, and $\mu = 10,000 \, cm^2/Vs$. (b) Same as in (a) but for the phase of transmission.
Figure 3.7: Retrieved (a) effective refractive index $n_e$ and (b) effective group index $n_g$ versus frequency. $S_1 = 5.5 \, \mu m$, $S_2 = 1.6 \, \mu m$, $\varepsilon_d = 3.5$, $\mu = 10,000 \, \text{cm}^2/\text{Vs}$, and $\mu_c = 1500 \, \text{meV}$. 
Here, \( \sigma_{\text{intra}} \) and \( \sigma_{\text{inter}} \) represent the intra- and inter-band transitions in the graphene layer and their expressions could be found in many recent studies \[109, 110\]. At low THz frequencies, where we have \( \sigma_{\text{intra}} \gg \sigma_{\text{inter}} \), \( \sigma_{S,G} \) could be approximated by a Drude model: 

\[
\sigma_{S,G}(\omega) \approx j \frac{q^2 \mu_c}{\pi \hbar (\omega + j \gamma)},
\]

where \( \omega \) is the angular frequency, \( q \) is the electron charge, \( h \) is the reduced Planck constant, \( \mu_c \) is the chemical potential of the doped graphene layer, and \( \gamma \) is the damping constant. It is assumed that the thickness of the graphene layer \( \delta = 1 \) nm; this choice was mainly motivated and justified by the seminal work of Vakil and Engheta \[109\]. Since \( \delta \) is much smaller than the wavelength at THz frequencies, graphene’s bulk conductivity can be simplified as \( \sigma_{V,G} = \sigma_{S,G}/\delta \).

Using Ampere’s law in stationary regime and Ohm’s law, one can calculate complex relative bulk permittivity of graphene as 

\[
\varepsilon_{V,G}(\omega) = 1 + j \frac{\omega_{G,p}^2 (\varepsilon_0 \omega)}{\omega (\omega + j \gamma/\hbar)}
\]

with the plasma frequency of graphene \( \omega_{G,p}^2 = \frac{q^2 \mu_c}{\delta \varepsilon_0 \pi \hbar^2} \). The damping constant used for graphene is given by \( \gamma = -\frac{e^2 v_f^2}{(\mu \mu_c)} \), where \( v_f = c/300 \) m/s is the Fermi velocity and \( \mu \) is the electron mobility. This expression clearly demonstrates the dependence of graphene layer’s complex permittivity \( \varepsilon_{V,G} \) on the chemical potential \( \mu_c \) and operating frequency \( \omega \). This dependence suggests that \( \mu_c \) can be varied to tune the spectral location and line-shape of the Fano resonance.

These material models are used in the finite element program COMSOL Multiphysics to carry out the simulations of electromagnetic wave interactions on the design presented in Figs. 3.1(a), 3.1(b), and 3.1(c). The results of these simulations are presented in the previous sections. These simulation results can also be “predicted” by the response of an RLC circuit as described in the next section.

### 3.5 RLC analytic model

The optical response of the proposed Fano resonator can be mathematically modeled using coupled oscillator equations. An RLC circuit model is used to replicate the
optical response of the Fano resonator [59].

In the circuit model, each of the dipolar SPPs induced on the gold frame and the graphene patch are represented by an RLC loop as shown in Fig. 3.8. Note that the additional third RLC loop in the circuit is needed to take into account the coupling from higher order SPPs induced on the gold frame and graphene patch beyond 12 THz. The loops are connected through three capacitors $C_{12}$, $C_{13}$, and $C_{23}$, which model the coupling between the different SPPs. This RLC circuit can be
mathematically represented as a system of three coupled equations:

\[
\begin{align*}
\Lambda_1 q_1 - \Omega_{12}^2 q_2 - \Omega_{13}^2 q_3 &= \varphi_1 \\
-\Omega_{12}^2 q_1 + \Lambda_2 q_2 - \Omega_{23}^2 q_3 &= \varphi_2 \\
-\Omega_{13}^2 q_1 - \Omega_{23}^2 q_2 + \Lambda_3 q_3 &= 0
\end{align*}
\] (3.2)

Here, \( q_i, i = 1, 2, 3, \) is the charge due to the steady state current \( I_i = j\omega q_i \) flowing in the loop indexed with \( i \). The term \( \Omega_{ij} = (L_i C_{x_i})^{-0.5} \), \( i, j = 1, 2, 3, i < j \), couples the three equations to each other, \( \Lambda_i = -\omega^2 + j\omega\gamma_i + \omega_i^2 \) represents the “self-coupling”, where \( \gamma_i = R_i/L_i \) is the damping coefficient, \( \omega_i = (L_i C_{x_i})^{-0.5} \), is the LC resonant frequency of the loop indexed with \( i \), and \( C_{x_i}^{-1} = C_1^{-1} + C_{12}^{-1} + C_{13}^{-1}, C_{x_2}^{-1} = C_2^{-1} + C_{12}^{-1} + C_{23}^{-1}, \) and \( C_{x_3}^{-1} = C_3^{-1} + C_{13}^{-1} + C_{23}^{-1} \). The terms \( \varphi_i = V_i/L_i \), \( i = 1, 2, \) on the right side of the system of equations (3.2) represent the excitation, i.e., the direct coupling from the incident field to the SPPs. The time average power drawn by the circuit is \( P = 1/2\Re[V_1 I_1^* + V_2 I_2^*] \) and this quantity should be equivalent to the extinction coefficient \( 1 - T \) of the Fano resonator. By minimizing the difference between \( P \) and \( 1 - T \) numerically, \( \omega_i, \gamma_i, \varphi_i, \) and \( \Omega_{ij} \) can be found. Once these coefficients are known, one can easily obtain the physical parameters, \( R_i, L_i, C_i, i = 1, 2, 3 \) and \( C_{12}, C_{13}, \) and \( C_{23} \), which describe the RLC circuit.

The mathematical model described by the system of equations (3.2) provides additional physical insight into the response of the Fano resonator. For example, \( \varphi_i, i = 1, 2, \) represent the amount of relative power each resonant mode receives from the incident electromagnetic field. Non-zero values of \( \varphi_i \) indicate that both modes have dipole moments along the polarization vector of the incident field and they can be directly excited. Variables \( \Omega_{12}, \Omega_{13}, \) and \( \Omega_{23} \) represent the amount of (energy) coupling between the modes. For example a high \( \Omega_{12} \) means that the coupling between \( D_1 \) and \( D_2 \) is strong, which indicates high transmittance \( T \) within the EIT region.
Table 3.1: Parameters of the RLC circuit model representing the Fano resonator with $S_1 = 5.5 \mu m$, $S_2 = 1.6 \mu m$, $\varepsilon_d = 3.5$, and $\mu = 10,000 \text{ cm}^2/\text{Vs}$ for various values of $\mu_c$ between 500 meV and 1500 meV. Units of $\omega_1$, $\omega_2$, $\omega_3$, $\Omega_{12}$, $\Omega_{13}$, and $\Omega_{23}$ are (meV) while the units of $\varphi_1$ and $\varphi_2$ are (mV/Hz).

This is demonstrated by an example as described next.

Parameters of the circuit with three loops is obtained by minimizing the difference between $P$ and $1 - T$ of the Fano resonator with $S_1 = 5.5 \mu m$, $S_2 = 1.6 \mu m$, $\varepsilon_d = 3.5$, and $\mu = 10,000 \text{ cm}^2/\text{Vs}$ for various values of $\mu_c$ between 500 meV and 1500 meV. The values of the extracted parameters are provided for each value of $\mu_c$ in Table 3.1. The effect of the increase in $\mu_c$ can be seen with a blue shift in the resonance frequency $\omega_2$ that corresponds to $D_2$. Additionally, a consistent increase in $\Omega_{12}$, which represents the strength of coupling between $D_1$ and $D_2$, is observed. As mentioned above, the increase in coupling strength, i.e., increase in $\Omega_{12}$ translates as increased $T$ within the EIT region [see Fig. 3.5(a)]. Note that as expected, increasing $\mu_c$ does not effect characteristics of $D_1$. As shown in Table 3.1, the resonant and damping frequencies, $\omega_1$ and $\gamma_1$, corresponding to $D_1$ remain unchanged.
3.6 Discussion and possible limitations

The proposed Fano resonator is equipped with the following properties that are superior to “classical” Fano resonators constructed using only noble metals:

(i) *Polarization Independence:* The design is polarization independent since it does not require excitation of higher order modes via symmetry breaking.

(ii) *Dynamic Tunability:* The spectral location and shape of the Fano resonance (and the EIT window) can be tuned by varying the chemical potential of the graphene patch. This can be dynamically achieved by applying a gate voltage to the graphene patch.

(iii) *Higher Group Index:* Group index extracted around the EIT window is higher than that reported in literature previously. This equips our design with a high sensitivity to the changes in the background medium’s refractive index.

It should be emphasized here that because gold’s intrinsic loss is higher than graphene’s, one would expect the overall loss in the hybrid resonator would increase, destroying the EIT. But it is observed that within the EIT region, where the destructive interference occurs, the radiation losses are suppressed. This is indeed why adding the gold frame to the system decreases the total losses within the EIT region instead of increasing them. The high transmittance values, which reach 80% as could be seen in Fig. 3.4(c), fully demonstrate this fact.

It should be noted here that the overall absorption is likely to increase because of the longer duration of interaction of light and dispersive “effective” material. However, since the thickness of the resonator is only 30 nm, the transmittance does not degrade and it stays around 40% at the frequency where \( n_g \) has the peak value.
3.7 Summary

To the best of our knowledge, our work is the first to report on EIT generated at THz frequencies using a hybrid graphene-gold structure. This novel design makes use of the fact that dipolar SPPs induced on graphene are much narrower than those induced on gold to induce the asymmetric Fano resonance shape in the spectrum. This concept is novel and has not been exploited before. The proposed resonator has potential applications in designing efficient electro-optic switches and ultra-sensitive bio-detectors that can be operated at THz frequencies. Our work also demonstrates the possibility of these via numerical simulations with realistic parameters.
Chapter 4

A Fano-Graphene field absorber

4.1 Introduction

There is an increased interest in designing perfect electromagnetic wave absorbers at terahertz (THz) frequencies since they are oftentimes an indispensable component in devices/systems utilized in biosensing, imaging, and communications [61]. Recently graphene has become one of the most attractive materials for designing THz-wave absorbers. The reasons are three-folds:

(i) A graphene layer can support surface plasmon polaritons (SPPs) at THz frequencies. Consequently absorption at the resonance frequency of the SPPs is significantly increased.

(ii) These frequencies can be dynamically tuned via biasing the graphene layer.

(iii) The absorption in an atomically thin graphene sheet is already very high, i.e., “2.3%” per layer.

However, considering its atomic thickness, a single layer of graphene remains practically transparent to THz waves and as a result the overall absorption is significantly reduced. To overcome this problem, patterned graphene layers (as opposed to uniform ones) have been designed [62, 63, 64, 125, 65]. Periodic patterns help to increase
the coupling of energy from the incident field to the SPPs \[62\] and therefore increase
the overall absorption. Absorber designs based on periodic arrays of graphene nano-
disks have been shown to fully absorb electromagnetic waves within the mid-infrared
spectrum\[62\]. The structured graphene in the form of micro-ribbons together with
the control of coherent interference effects from back reflector permits complete ab-
sorption within the same frequency range \[64\].

From a practical point of view, the bandwidth of absorption at THz frequencies
is important for many of the applications mentioned above \[61\]. But unfortunately,
achieving broadband absorption at THz frequencies still remains a challenging task
\[126\]. The current bandwidth of operation in metal-based plasmonic absorbers is
limited to only a few THz (see \[126, 127, 128, 129, 130, 131\] in Table 4.1). This
is attributed to the narrow bandwidth of SPPs generated on metallic surfaces at
nanoscales, which are used as a mechanism to achieve absorption. The damping on
graphene layer is even smaller than that on the metal surface, therefore graphene
SPPs are also narrowband resulting in a bandwidth of absorption smaller than 1.8
THz (see \[62, 63, 64, 125, 65\] in Table 4.1).

In this chapter, an absorber design operating at THz frequencies is proposed. The
design makes use of three mechanisms:

(i) The asymmetric pattern on the graphene layer(s) allows for generation of higher
order SPP modes with resonance frequencies that can be tuned via electrical bi-
asing. The interference between the higher order modes leads to the generation
of asymmetric lineshape characterized by Fano resonance.

(ii) Several patterned graphene layers biased at different voltages backed with di-
electric substrates are stacked on top of each other.

(iii) Graphene’s damping factor is increased by lowering its electron mobility to
1000 cm$^2$/Vs.
It should be emphasized here that mechanisms (i) and (ii) are being used for the first time in absorber design. The use of an asymmetric pattern results in a quadrupolar SPP, which generates electromagnetically induced absorption by destructively interfering with the fundamental dipolar SPP at THz frequencies [132, 133]. Even though the resulting design is polarization dependent, it has drastically increased the bandwidth of near-unity absorption in comparison with graphene absorbers designed to operate with only dipolar mode [64]. The idea of biasing graphene layers at different voltages allows for generation of SPPs at different frequencies and increases the “chance” of destructive interference between reflected and transmitted fields at different graphene layers. Additionally, even though the mechanism (iii) is not novel, increasing graphene’s damping factor broadens the bandwidth of plasmonic resonances and hence that of the absorption as well [134, 108]. It is demonstrated numerically that the combination of these three mechanisms significantly increases the bandwidth of the proposed absorber in comparison with the designs listed in Table 4.1.

4.2 Design details and results

4.2.1 Design

The principle behind achieving near-unity absorption is the destructive interference of fields reflected from (multiple) layers of (lossy) impedance surfaces, dielectric substrates, and a fully reflective ground plane. The ground plane does not allow any fields to be transmitted and the only possible reflection path is suppressed through the destructive interference of the fields. Obviously, this leads to a highly enhanced absorption [135, 136].

Based on the above principle, the absorber shown in Fig. 4.1 is designed. Three impedance surfaces (at 1st, 2nd and 3rd interface respectively) are patterned layers of
<table>
<thead>
<tr>
<th>Reference</th>
<th>Near-Unity Absorption Bandwidth</th>
<th>Normalized BW/$f_0$ x100</th>
<th>Material</th>
</tr>
</thead>
<tbody>
<tr>
<td>[62]</td>
<td>32.4 THz – 32.6 THz = 0.2 THz</td>
<td>0.6</td>
<td>Graphene</td>
</tr>
<tr>
<td>[63]</td>
<td>1.6 THz – 2.2 THz = 0.6 THz</td>
<td>31.5</td>
<td>Graphene</td>
</tr>
<tr>
<td>[64]</td>
<td>3.5 THz – 3.6 THz = 0.1 THz</td>
<td>2.8</td>
<td>Graphene</td>
</tr>
<tr>
<td>[125]</td>
<td>1.25 THz – 1.3 THz = 0.05 THz</td>
<td>3.9</td>
<td>Graphene</td>
</tr>
<tr>
<td>[65]</td>
<td>2.2 THz – 4 THz = 1.8 THz</td>
<td>58.0</td>
<td>Graphene</td>
</tr>
<tr>
<td>[126]</td>
<td>0.88 THz – 0.96 THz = 0.08 THz</td>
<td>8.6</td>
<td>Gold</td>
</tr>
<tr>
<td>[127]</td>
<td>8 THz – 11.7 THz = 3.7 THz</td>
<td>37.5</td>
<td>Gold</td>
</tr>
<tr>
<td>[128]</td>
<td>0.48 THz – 0.51 THz = 0.03 THz</td>
<td>6.0</td>
<td>Gold</td>
</tr>
<tr>
<td>[129]</td>
<td>4.5 THz – 5.5THz = 1 THz</td>
<td>20.0</td>
<td>Gold</td>
</tr>
<tr>
<td>[130] *</td>
<td>1.4 THz – 1.5 THz = 0.1 THz, 2.8 THz – 3 THz = 0.2 THz</td>
<td>6.9, 6.8</td>
<td>Gold</td>
</tr>
<tr>
<td>[131] *</td>
<td>2.8 THz – 2.9 THz = 0.1 THz, 4.9 THz – 5.1 THz = 0.2 THz</td>
<td>3.5, 4.0</td>
<td>Gold</td>
</tr>
<tr>
<td>Present Study</td>
<td>4.7 THz – 11.6 THz = 6.9 THz</td>
<td>84.6</td>
<td>Graphene</td>
</tr>
</tbody>
</table>

Table 4.1: Comparison between bandwidths of 90% absorption at THz frequencies. Studies marked with * describe multiple bands of absorption above 90%.
Figure 4.1: The schematic diagram of the proposed absorber with three layers of graphene.
graphene (Section 4.2.2) separated by dielectric substrates with relative permittivity $\varepsilon_r = 2.5$ and thickness $d_1$, $d_2$, and $d_3$, respectively. The reflector at the bottom is gold. The electrostatic biasing of each graphene layer is done via applying a gate voltage by placing conductive contacts between each layer and the gold reflector (electrostatic ground). The bias allows for controlling the chemical potential $\mu_c$ of each graphene layer independently [137]. It should be noted here that the biasing method used here eliminates the need for designing transparent electrodes [62, 60, 98] and reduces the overall complexity of the design significantly.

The absorber in Fig. 4.1 is assumed to be excited with an incident electromagnetic plane wave traveling in $y$-direction with the electric field vector polarized along $x$-direction. Using the transmission line model [135] to take into account the field interactions between graphene layers, the absorption associated with the multilayered design is expressed [138]

$$ A = 1 - |\Gamma_1|^2, \quad (4.1) $$

where

$$ \Gamma_1 = r_{12} + \frac{t_{21}t_{12} \Gamma_2 e^{-i2\phi_1}}{1 - r_{21}\Gamma_2 e^{-i2\phi_1}} $$
$$ \Gamma_2 = r_{23} + \frac{t_{32}t_{23} \Gamma_3 e^{-i2\phi_2}}{1 - r_{32}\Gamma_3 e^{-i2\phi_2}} $$
$$ \Gamma_3 = r_{34} + \frac{t_{43}t_{34} r_{45} e^{-i2\phi_3}}{1 - r_{43} r_{45} e^{-i2\phi_3}}. \quad (4.2) $$

Here, $\Gamma_i$, $i = 1 : 3$ represent the total reflection coefficients at the first, second, and third interfaces, $\phi_i = k n d_i$ are the phase lengths across the first, second, and third dielectric substrates, $n = \sqrt{\varepsilon_r}$ is their refractive index, and $t_{ij}$ and $r_{ij}$ represent individual transmission and reflection coefficients of the impedance surfaces (See Fig. 2). Several comments about the mathematical model described by Eqs. 4.1 and 4.2...
are in order:

(i) Reflection and transmission coefficients of the interfaces with impedance surfaces, $t_{ij}$ and $r_{ij}$ are computed using a full-wave numerical method as described in Section 4.2.2 (Fig. 4.2).

(ii) It is assumed here that the gold ground plane is a perfect reflector, i.e., $r_{45} = -1$ and therefore the total transmission through the structure is zero.

(iii) It has been shown before in [135] that transmission line model used here is valid when the capacitive coupling between two graphene layers is small. This means that, for Eqs. 4.1 and 4.2 to produce accurate results, near field coupling between two layers should be small. Indeed, for the frequency band considered here and dimensions of the periodic pattern on the graphene layers (Section 4.2.2) (Fig. 4.3), the near fields stay tightly bounded to the graphene surface. Therefore, restricting substrate thicknesses to $d_{1,2,3} \geq 0.5 \mu m$ reduces the capacitive coupling and makes the mathematical model described by Eqs. 4.1 and 4.2 accurate. It should also be noted here that the transmission line model is validated via comparison by a full-wave numerical method.

4.2.2 Patterned graphene layer

The purpose of using patterned graphene layers in the design of the multilayered absorber, which is shown in Fig. 4.1 and described in Section 4.2.1, is to increase the bandwidth of near-unity absorption. The pattern on the layers is generated by repeating a unit cell with a rectangular void periodically in $x$ and $y$-directions (Fig. 4.3). It should be emphasized here that void is located asymmetrically (with respect to the excitation) to generate higher order plasmon modes on the graphene surface [15, 24].
Transmission and reflection coefficients, $t_{ij}$ and $r_{ij}$, which are required by equation 4.2, are evaluated using the fields scattered from the patterned graphene layer under the same excitation that is shown in Fig. 4.1 and described in Section 4.2.1. Scattered fields are computed using the commercially available finite element simulator COMSOL [95]. In these simulations, the complex (bulk) permittivity of graphene is modeled using

$$\varepsilon_G(\omega) = 1 + \frac{j\sigma_G(\omega)}{\varepsilon_0\omega} \approx \frac{-\omega_P^2}{\omega(\omega + j\gamma/\hbar)},$$

(4.3)

where $\sigma_G$ represents graphene’s bulk conductivity, $\omega_P^2 = (q^2\mu_c)/(\Delta\varepsilon_0\pi\hbar^2)$ is its equivalent plasma frequency, $\Delta$ is the thickness of the layer, $q$ is the electron charge, $\hbar$ is the reduced Plank’s constant, $\mu_c$ is the chemical potential, $\gamma = -(q\hbar v_f^2)/(\mu\mu_c)$ is the damping constant, $\mu$ is the electron mobility, $v_f = c/300\text{m/s}$ is the Fermi velocity, and $c$ is the speed of light in free space.

First, reflectance, transmittance, and absorption spectra of the patterned graphene layer are computed for $\mu_c = 1000\text{meV}$ and $\mu = 10,000\text{cm}^2/\text{Vs}$. Two dominant reso-
nant modes are clearly identified in the spectra provided in Fig. 4.4(a). As expected, the geometrical asymmetry results in generation of a higher order mode. Surface charge distribution computed at 10 THz on the graphene unit cell [Fig. 4.4(b)] clearly demonstrates that this mode is quadrupolar. It is originally dark, but, because of the unit cell’s geometrical asymmetry, it becomes dipole-active permitting efficient energy coupling from the incident field. The characteristic asymmetric Fano lineshape and a narrow electromagnetically induced transparency (EIT), which result from destructive interference of this mode with the dipolar mode, are clearly observed in the reflectance spectra around 9 THz. It is also observed in Fig. 4.4(a) that the reflectance of the quadrupolar resonance is stronger compared to that of the dipolar resonance. Furthermore, it is noticed that two additional relatively weak higher order modes are observed beyond 15 THz.

Equation 4.3 shows that graphene’s dielectric permittivity $\varepsilon_G$ depends on its chemical potential $\mu_c$. As a natural consequence, graphene layer’s electromagnetic response can be controlled by varying $\mu_c$. It should be noted here that varying $\mu_c$ is equivalent to varying the bias voltage of the layer \[109\]. Graphene layer’s reflectance and transmittance spectra are computed for $\mu = 10,000 \text{cm}^2/\text{Vs}$ and varying values of $\mu_c$. 

Figure 4.3: The graphene unit cell with an asymmetric void with its dimensions.
Figure 4.4: (a) Transmittance, reflectance, and absorption of a single layer of patterned graphene for $\mu_c = 1000$ eV and $\mu = 10,000$ cm$^2$/Vs. (b) Normalized surface charge density distribution on the unit cell at the frequency points identified on the curve. (c) Transmittance and (d) reflectance spectra of the patterned graphene layer for varying values of $\mu_c$. The color bar represents the value of transmittance in (c) and reflectance in (d).
between 100 meV and 1000 meV. Results are presented in Figs. 4.4(c) and 4.4(d), respectively. It can be deduced from equation 4.3 that higher values of $\mu_c$ increase $\varepsilon_G$ and make the graphene layer a better scatterer, i.e., more reflective. This is demonstrated by Fig. 4.4(d), where the maximum reflectance is clearly higher for higher values of $\mu_c$. Also, Figs. 4.4(c) and 4.4(d) show that increasing $\mu_c$ blue-shifts the quadrupolar and dipolar resonances and the EIT band as a consequence. Controllability of the reflectance and transmittance through voltage biasing opens up possibility of increasing the absorption bandwidth by stacking graphene layers biased at different voltages as described in Sections 4.2.4 and 4.2.5.

4.2.3 One-layer graphene absorber

For this design, it is assumed that the graphene layer and the gold reflector are located at the first and second interfaces, respectively (Fig. 4.2). The absorption of the design is computed using equation 4.1 where now $\Gamma_1$ is obtained by setting $\Gamma_2 = r_{23} = -1$ in equation 4.2. The design parameters to be selected are the thickness of the dielectric substrate $d_1$, chemical potential and electron mobility of the graphene layer, $\mu_c$ and $\mu$, respectively. The dielectric substrate could be thought of as a Fabry-Perot interferometer terminated at its ends with a gold reflector and a partially reflective graphene layer [138]. Interferometer parameters free spectral range $\text{FSR} = c/2nd_1$ and finesse $= \text{FSR}/\text{FWHM}$ represent the frequency difference between successive resonant transmission peaks and their sharpness, respectively [139]. Similar to this concept, here the FSR and finesse of the dispersive and lossy cavity, which is formed by the dielectric substrate terminated by a graphene layer on one end, can be used to characterize its absorption properties. Clearly, $d_1$ should be selected carefully since it determines the resonance locations, where maximum absorption occurs. It also has an effect on the bandwidth of absorption since the patterned graphene layer supports two peaks in the reflectance spectrum with different bandwidths.
Figure 4.5: (a) Absorption spectra of the one-layer design with varying values of $d_1$ and various values of $\mu_c$. (b) Absorption spectra of the one-layer design with varying values of $\mu_c$ and various values of $d_1$. The color bar represents the value of absorption. (c) Absorption of the one-layer design with $\mu_c = 500$ meV and $d_1 = 100 \mu m$ exhibiting multiple resonances due to smaller FSR $= 0.95$ THz.
Figure 4.6: (a) Absorption spectra of the one-layer design with varying values of $d_1$ and various values of $\mu$. The color bar represents the value of absorption. (b) Relationship between the absorption maximum and the bandwidth of 90% absorption as a function of $\mu$. (c) The absorption spectra of the one-layer design with $\mu = 1000 \text{ cm}^2/\text{Vs}$ and $d_1 = 5 \mu\text{m}$.
It was shown in Section 4.2.2 that the graphene layer becomes more reflective, i.e., dipolar and quadrapolar resonances in reflectance spectrum become stronger, when \( \mu_c \) is increased. As a consequence, the dielectric substrate maintains a greater finesse; alike the finesse of a laser cavity terminated with highly reflecting mirrors. As \( \mu_c \) is lowered, finesse of the dielectric layer decreases and dipolar and quadrupolar resonances start overlapping to merge together. The above statements are clearly shown in Figs. 4.5(a) and 4.5(b), where the absorption spectra of the one-layer design is provided for various values of \( d_1 \) and \( \mu_c \). For \( d_1 = 100 \mu m \), FSR = 0.95 THz, a relatively smaller value, which makes the multiple resonances in the absorption spectrum more visible [see Fig. 4.5(c)]. Note that these absorption resonances are dispersive unlike the modes of a lasing cavity. Also, note that the multiple (narrowband) resonances are not desirable to achieve broadband (flat top) absorption spectrum. Smaller values of \( d_1 \) are more suitable for this purpose.

Next, the effect of \( \mu \) on the absorption spectrum of the one-layer design is characterized. Figure 4.6(a) presents absorption spectra computed for various values of \( \mu \) and \( d_1 \). The figure clearly shows that for a given value of \( d_1 \), decreasing \( \mu \) (i.e. high losses) significantly increases the bandwidth of absorption. But at the same time, the maximum value of absorption also decreases [Fig. 4.6(b)]. It should also be noted here that the presence of multiple resonances due to the decrease in FSR for large values of \( d_1 \) is clearly identified in Fig. 4.5(c).

Based on the results presented above, we choose:

(i) \( d_1 = 5 \mu m \) to avoid separated multiple bands of absorption due to Fabry-Perot cavity resonances,

(ii) \( \mu_c = 1000 \text{meV} \) to make dipolar and quadrapolar modes overlap and increase the bandwidth of absorption, and

(iii) \( \mu = 1000 \text{cm}^2/\text{Vs} \) to ensure absorption is near-unity without sacrificing too
much from bandwidth.

The absorption spectrum of the one-layer design with these parameters is computed and shown in Fig. 4.6(c). The bandwidth of 90% absorption reaches approximately 3.7 THz making the absorber suitable for practical applications. Introducing additional layers as described next in Sections 4.2.4 and 4.2.5 can further increase the bandwidth.

4.2.4 Two-layer graphene absorber

For the two-layer design, the two graphene layers and the gold reflector are located at the first, second, and third interfaces, respectively (Fig. 4.2). The absorption of the design is computed using equation 4.1, where now $\Gamma_1$ and $\Gamma_2$ are obtained by setting $\Gamma_3 = r_{34} = -1$ in equation 4.2 (Fig. 4.2). To simplify the problem of selecting design parameters, the chemical potentials of the first and second graphene layers are set to $\mu_c = 1000$ meV and $\mu_c = 700$ meV, respectively and electron mobility of both layers is set to $\mu = 1000$ cm$^2$/Vs. Then, the design parameters to be selected are the thicknesses of the dielectric substrates, $d_1$ and $d_2$. The absorption spectrum is computed for various values of $d_1$ and $d_2$; the results are presented in Figs. 4.7(a) and 4.7(b). These figures clearly show that largest bandwidth of absorption can be obtained between 4 THz and 12 THz and for smaller values of $d_1$ and $d_2$. Keeping those in mind, to be able to maximize the bandwidth,

$$\text{FOM}(d_1, d_2) = \int_{4 \text{THz}}^{12 \text{THz}} A \, df$$

is defined as a figure of merit and values of $d_1$ and $d_2$ that maximize it are sought for. FOM is computed for various values of $d_1$ and $d_2$ and plotted in Fig. 4.8(a). The figure shows that FOM has a maximum for $d_1 = 0.5 \mu m$ and $d_2 = 5.45 \mu m$. The absorption spectrum of the two-layer design with these values is plotted in Fig. 4.8(b).
Figure 4.7: (a) Absorption spectra of the two-layer design with (a) varying values of $d_1$ and various values of $d_2$ and (b) varying values of $d_2$ and various values of $d_1$. The color bar represents the value of absorption in (a) and (b).
Figure 4.8: FOM of the two-layer design as a function of $d_1$ and $d_2$. (b) The absorption spectra of the two-layer design with $d_1 = 0.5 \mu m$ and $d_2 = 5.45 \mu m$. The color bar represents the absolute value of FOM.
Figure 4.9: The absorption spectra of the three-layer design with \( d_1 = 0.67 \mu m \), \( d_2 = 0.5 \mu m \), and \( d_3 = 4.78 \mu m \).

The bandwidth of the 90\% absorption reaches 5.8 THz.

### 4.2.5 Three-layer graphene absorber

For the three-layer design, three graphene layers and the gold reflector are located at the first, second, third, and fourth interfaces, respectively (Fig. 4.2). The absorption of the design is computed using equation 4.1 (Fig. 4.2). The chemical potential of the graphene layers are set to \( \mu_c = 1000 \) meV, \( \mu_c = 700 \) meV, and \( \mu_c = 500 \) meV, respectively and the electron mobility of all three layers is set to \( \mu = 1000 \) cm\(^2\)/Vs.

The design parameters to be selected are the thicknesses of the dielectric substrates,
It is found that $d_1 = 0.67 \mu m$, $d_2 = 0.5 \mu m$ and $d_3 = 4.78 \mu m$ maximize

$$FOM(d_1, d_2, d_3) = \int_{4 \text{THz}}^{12 \text{THz}} A(df)$$

The absorption spectrum of the three-layer design with these values is plotted in Fig. 4.9. The bandwidth of 90% absorption reaches 6.9 THz.

### 4.3 Discussion and possible limitations

It is numerically demonstrated that with only three layers, bandwidth of 90% absorption can be extended upto 7 THz, which is drastically larger than only few THz of bandwidth that can be achieved with existing metallic/graphene absorbers [62, 63, 64, 125, 65, 126, 127, 128, 129, 130, 131]. However, two limitations that might hinder the potential use of such absorber are polarization dependence of the resonator response and the difficulty to achieve the required biasing for the multilayer graphene in order to get the desired absorption characteristics. All these limitation shall be addressed in the future research work.

### 4.4 Summary

An ultra-broadband multilayered graphene absorber that operates at THz frequencies is described. The graphene layers are asymmetrically patterned to generate quadrupolar SPPs that destructively interfere with the dipolar ones. The patterned graphene layers biased at different voltages backed-up with dielectric substrates are stacked on top of each other. Additionally, graphene’s damping factor is increased by lowering its electron mobility to 1000 cm$^2$/Vs. Numerical experiments demonstrate that combination of these three mechanisms has significantly increased the design’s bandwidth of operation: 6.9 THz bandwidth is obtained for 90% absorption.
Chapter 5

A nonlinear three-state plasmonic resonator

5.1 Introduction

The support of highly localized and strong fields in the vicinity of metal/dielectric interfaces due to surface plasmon modes allows for the drastic enhancement of weak nonlinear processes [140] [50]. This concept of plasmonic-enhanced nonlinearity has recently been used in designing photonic devices with bi-stable responses. The nonlinear bi-stability, i.e., the reversible change in the response of a device, enables ultrafast changes in the output due to variations in the input [50] suggesting possible applications in switching. Additionally, the presence of two-states in the output can be used in digital logic systems. Indeed, static random access memory applications, which make use of nonlinearities in output states of photonic devices, are under development [50]. Recent work on nonlinear photonic devices has focused on using bi-stability to switch on and off certain characteristics of optical nanoantennas, cloaks, and negative and near-zero refractive index materials [67] [69] [68] [70] [71] using self-modulation schemes. Along the same lines, a step-like transmission, similar to nonlinear bi-stability, has been obtained through an asymmetric Fano resonance generated by a Kerr layered/grating structure [141]. Similarly, a one-dimensional grating
consisting of alternating layers of dielectric and chalcogenide glass has been used to obtain bi-stability in the reflected field \[142, 143, 144\]. The field localization on a two-dimensional photonic crystal has also been exploited to generate bi-stability for a low input power level but at a narrow bandwidth \[145\].

Oftentimes, singly resonant photonic structures with high \(Q\) factors are used for enhancing weak nonlinear processes introduced by medium properties. This reduces the input power level required by the design to operate within the nonlinear region since it scales with \(1/Q^2\) \[142, 143, 144\]. However, typically, high \(Q\) factors come at the cost of reduced bandwidth of operation. Lossless dielectric cavities \[51, 53\] or under-damped (lossy) singly resonant plasmonic resonators \[67, 68\] have been used for enhancing nonlinearities but with a limited bandwidth of operation.

The significant improvements that come with using three-state switches (instead of their two-state counterparts) for communications and computing in the field of digital electronics have been well-understood. In data communication, the process of line coding converts the raw digital data to digital signals \[2\]. Several multi-level line coding schemes, which benefit from the use of three-state output, have been developed; these include the well-known 4B/3T and 8B/6T encoding schemes \[2\]. An example of 8B/6T line coding scheme is described in Fig. 5.1(a): 8-bits (1 byte) of binary data are encoded to 6-bits of ternary digital signal. A signal described using ternary states instead of binary ones helps in better synchronization and increasing the data rate of the communication system \[2\]. In Fig. 5.1(b) a three-state logic gate is described; this type of gates are used in digital computing systems whenever multiple devices are connected together through a bus \[3\]. Here, the additional “enable” input is responsible for connecting or isolating the device output from the rest of the system, which cannot be achieved with gates that support standard two state output. Three-state logic gates are essentially used in computing and communication applications to provide time-division multiplexing for several devices connected to a
Figure 5.1: (a) A example of 8B/6T encoding that uses three states to describe the binary data [2]. (b) Schematic diagram of a three-state logic device and its truth table. The output gate supports a high impedance state in addition to the 0 and 1 logic levels [3]. (c) Example use of a three-state logic gate where several devices share a single bus waveguide.
single channel. No useful communication can take place if all the devices simultaneously try to communicate their digital data over the bus waveguide. However, if the devices support three-state outputs, where the lowest state corresponds to an open circuit (high impedance state) the devices could communicate to the bus-waveguide (one device at a time), [Fig. 5.1(c)] [3]. It should be clear from the discussion here that, for both of the examples described in Figs. 5.1(a) and 5.1(b), the device support with three-state output is essential. In digital electronics, three-state logic devices are realized with TTL or CMOS technology [3].

Similarly, all-optical communication and computing systems can benefit from advantages that come with three-state switches. The optical implementation of three-state switches making use of Kerr nonlinearity has previously been achieved using photonic bandgap structures [146 147 148] and coupled waveguide-cavity resonators [149].

In this chapter, a plasmonic resonator that supports three states in its output at frequencies ranging from infrared to optical parts of the spectrum is designed for that purpose. The optical response required for three-state output is achieved by enhancing nonlinearities of a Kerr medium through multiple higher order plasmons excited on resonator’s metallic surfaces. Exploitation of multiple plasmons equips the proposed resonator with characteristics that cannot be obtained using existing nonlinear device designs that make use of single-mode Lorentzian resonances:

(i) It supports nonlinear response at multiple bands of frequencies, which cumulatively increases the bandwidth of operation.

(ii) It supports nonlinear tri-stable output characteristics that cannot be achieved using existing Kerr nonlinear devices with bi-stable output states [68 142 143 144].
Figure 5.2: Schematic of the proposed resonator. The gap between the gold frame and the rod is highlighted in red color.

5.2 Design details and results

5.2.1 Design

To achieve broadband multi-stable characteristics in the design output three different criteria are set for a plasmonic nanostructures:

(i) Ability to generate higher order modes.

(ii) Support of high and uniform fields inside a smaller region where the Kerr-nonlinear material is located.

(iii) Ability to operate at normal incidence at optical frequencies. The plasmonic
Figure 5.3: Gap electric field enhancement $|E_g|/|E_0|$ computed at various values of $\varepsilon_g$ at a band of frequencies between 175 THz and 500 THz. Insets show normalized surface charge density induced on the resonator surface at three different frequencies.

The proposed resonator design consists of a square gold frame and a rectangular gold rod (Fig. 5.2). The geometry dimensions shown in the figure are $R_1 = 120$ nm, $R_2 = 90$ nm, $L = 50$ nm, $W = 20$ nm, $g = 2$ nm, and $t = 10$ nm. It should be noted here that selection of $g = 2$ nm ensures that a strong and (essentially) uniform electromagnetic field is generated inside the gap; this field is denoted by $E_g$. The gap between the frame and the rod is filled with a material with relative permittivity $\varepsilon_g$. The intrinsic nonlinearity of gold is assumed to be negligible and the tabulated values of its permittivity are used in the simulations [96]. The resonator is excited by a normally incident plane wave with electric field polarized parallel to the rod (Fig. 5.2). The input intensity of this field is denoted by $I_0$. It should be noted here that multiple higher order surface plasmon resonances are induced as a result of the broken geometrical symmetry (with respect to the excitation) [24, 15, 59, 60] obtained by shifting the rod along the horizontal axis of the frame. This shift allows
the incident field to couple to the higher order surface plasmons.

5.2.2 Linear simulations

To demonstrate the presence of multiple (higher order) surface plasmons in the response of the resonator, enhancement $|E_g|/|E_0|$ is computed at frequencies between 175 THz and 500 THz for $I_0 = 21 \text{ W/cm}^2$ and various values of $\varepsilon_g$. Enhancement $|E_g|/|E_0|$ is plotted against frequency in Fig. 5.3. The resonance frequencies of the plasmons are clearly identified as three well-separated peaks in the figure. It is well-known that the bi-stability is a result of the fact that the spectral location of a single plasmonic resonance is sensitive to variations in $\varepsilon_g$. Similarly, as shown in Fig. 5.3, multiple plasmonic resonances are also sensitive to variations in $\varepsilon_g$. This suggests that when the gap is filled with a nonlinear medium, i.e., when $\varepsilon_g$ changes nonlinearly with $E_g$ (or $I_0$), the multiple peaks in the $|E_g|\varepsilon_g$ curves will provide a mechanism for the generation of multi-band tri-stability. This is demonstrated next.

5.2.3 Nonlinear simulations

For the “nonlinear” simulations of the resonator, the gap is assumed to be filled with Ag-BaO, which is modeled as a third order nonlinear $\chi^{(3)}$ Kerr material [150]. Its relative permittivity is given by

$$\varepsilon_g = \varepsilon_L + \chi^{(3)}|E_g|^2, \quad (5.1)$$

where $\varepsilon_L = 2.52$ is the linear component and $\chi^{(3)} = 6.72 \times 10^{-18} \text{ m}^2/\text{V}^2$ is the third order nonlinear susceptibility.

The nonlinear simulation is carried out using the well-known graphical method [151]. At a given frequency and $I_0$, “linear” simulations are carried out to compute $E_g$ for various values of $\varepsilon_g$. Then, $|E_g|$ is plotted against $\varepsilon_g$. For linear simulations, since $|E_g|$
Figure 5.4: An example of how the graphical method is used for computing the nonlinear response of the resonator. Frequency is 410 THz and only $|E_g| - \varepsilon_g$ curves for $I_0 = 19.5$ MW/cm$^2$ and $I_0 = 3.74$ GW/cm$^2$ are plotted for demonstration. The intersection points on the graph represent the solution of the nonlinear simulation.

scales linearly with $\sqrt{I_0}$, additional curves for different values of $I_0$ are obtained by simply shifting the initial $|E_g| - \varepsilon_g$ curve. The intersection points of these curves with the curve of the nonlinear relation in Eq. (5.1) are found. These intersection points defined by values of $I_0$, $|E_g|$, and $\varepsilon_g$ are the solutions to the nonlinear simulation.

The graphical method can be explained better with an example (Fig. 5.4). The nonlinear simulation of the resonator is carried out at 410 THz. First, for $I_0 = 19.5$ MW/cm$^2$, $E_g$ is computed for a set of values of $\varepsilon_g$ between 1 and 18, and the $|E_g| - \varepsilon_g$ (green) curve is plotted. Then, the $|E_g| - \varepsilon_g$ (blue) curve for $I_0 = 3.74$ GW/cm$^2$ is obtained by simply scaling the curve for $I_0 = 19.5$ MW/cm$^2$. The curve for $I_0 = 19.5$ MW/cm$^2$ intersects the (black) curve of the nonlinear relation in Eq. (5.1) at three different points. The middle point corresponds to the solution for the unstable branch of the bi-stability. Similarly, the curve for $I_0 = 3.74$ GW/cm$^2$ has five intersection points (Fig. 5.4) that correspond to a combined bi- and tri-stability.

Next, the graphical method described above is used to find the response of the
Figure 5.5: Extinction CS spectrum of the resonator with nonlinear $\epsilon_g = \epsilon_L + \chi^{(3)}|E_g|^2$, $\epsilon_L = 2.52$, $\chi^{(3)} = 6.72 \times 10^{-18}$ m$^2$/V$^2$ and with linear $\epsilon_g = 2.52$, which is computed for $I_0 = 0.22$ GW/cm$^2$ and $I_0 = 21$ W/cm$^2$, respectively. Figure 5.5 compares the extinction cross section (CS) spectrum of the proposed nonlinear resonator and a linear resonator with its gap loaded with a material with $\epsilon_g = 2.52$ for $I_0 = 0.22$ GW/cm$^2$ and $I_0 = 21$ W/cm$^2$, respectively. It is clearly seen that the high input intensity self-modulates the response of the nonlinear resonator and four bi-stability regions are clearly identified in the extinction CS spectrum.

At the frequency 410 THz, the two steps of graphical method applied in the above example in Fig. 5.4 [scaling of the curves and finding their intersections with the curve of Eq. (5.1)] are repeated for a set of values of $I_0$ between 2 MW/cm$^2$ and 10 GW/cm$^2$. Figure 5.6(a) plots $\epsilon_g$ against $I_0$. Let $T_i$, $i = 1, ..., 6$, represent the thresholds of $I_0$ for stable resonator operation. It is clearly shown in Fig. 5.6(a) that between $T_1$ and $T_2$, $\epsilon_g$ forms a connected double S chain representing the bi-stability in the response of the resonator. Between $T_3$ and $T_6$ both bi- and tri-stability are observed. Note that the tri-stability condition is achieved when three stable states are simultaneously
Figure 5.6: Near-field response of the resonator with nonlinear permittivity $\varepsilon_g = \varepsilon_L + \chi^{(3)} |E_0|^2$, $\varepsilon_L = 2.52$, $\chi^{(3)} = 6.72 \times 10^{-18} \text{ m}^2/\text{V}^2$. $\varepsilon_g$ as a function of $I_0$ at (a) 410 THz. Extinction CS as a function of $I_0$ at (b) 410 THz.
Figure 5.7: Near-field response of the resonator with nonlinear permittivity $\varepsilon_g = \varepsilon_L + \chi^{(3)} |E_0|^2$, $\varepsilon_L = 2.52$, $\chi^{(3)} = 6.72 \times 10^{-18}$ m$^2$/V$^2$. $\varepsilon_g$ as a function of $I_0$ at (a) 498 THz. Extinction CS as a function of $I_0$ at (b) 498 THz.
generated within the same range of $I_0$.

The nonlinear simulation described above is repeated at 498 THz. Figure 5.7(a) plots $\varepsilon_g$ against $I_0$. A small bi-stable region between $T_3$ and $T_4$ is added on top of a broader bi-stable region between $T_1$ and $T_2$, making this region exhibit tri-stability.

It should be noted here that the resonator’s geometry is designed to ensure that the specific features visible in its far-field originate from its near-field response [152]. As a consequence, the effects of nonlinearity on $E_g/\varepsilon_g$ as shown in Figs. 5.6(a) and 5.7(a) are expected to appear in the resonator’s far-field response. Indeed, bi-, multi-, bi-, and tri-stability are achieved in the extinction CS spectrum of the resonator. This is clearly demonstrated in Figs. 5.6(b) and 5.7(b), where the extinction CS of the resonator is plotted against $I_0$ at 410 THz and 498 THz, respectively. At 410 THz, the extinction CS forms an oval shape for the initial bi-stability between $T_1$ and $T_2$ and a connected double inverted S chain in the form of multi-bi- and tri-stable states between $T_3$ and $T_6$ [Fig. 5.7(a)]. Similarly, Fig. 5.7(b) shows a tri-stable extinction CS between $T_3$ and $T_4$ at 498 THz. In this case, a small bi-stable region between $T_3$ and $T_4$ is added on top of a broad bi-stable region between $T_1$ and $T_2$, making this region exhibit tri-stability. Figures 5.6(a) and 5.7(b) and 5.6(b) and 5.7(b) also show that multi-bi-stability and tri-stability states are excited at higher values of $I_0$ between 1 GW/cm$^2$ and 10 GW/cm$^2$ in comparison with values of $I_0$ required for bi-stable only operation.

5.3 Discussion and possible limitations

Figure 5.5 clearly demonstrates the multi-band characteristics of the proposed resonator’s nonlinear response. Compared to conventional Lorentzian based resonators [68, 142, 143, 144], the proposed design, can be made bi-stable within all these frequency regions without any modifications on the geometry. Consequently, the bandwidth
of operation for nonlinear functionalities including switching can be significantly increased.

In addition to optical bi-stability, the multi-stability supported by the proposed resonator in the forms of multi-bi-stability and tri-stability in Figs. 5.6(a)-(b) provides a mechanism for realizing multi-state output for optical switching and memory access applications as described next. The stable branches within the tri-stability region ($T_2 < I_0 < T_3$) are highlighted in Fig. 5.8(a). In this figure, branches between output intensity levels $O_1 - O_2$, $O_3 - O_4$, and $O_5 - O_6$ are assigned to output states 1, 2 and 3, respectively. The state flow diagram in Fig. 5.8(b) describes the states of all-optical switching and memory access applications that can be achieved using the proposed resonator. The switching behavior requires transition among the three states of flow diagram (blue and yellow arrows) [Fig. 5.8(b)]. The transition (or switching) to another state requires the corresponding input intensity $I_0$ to be varied accordingly (shown on the arrows of diagram). For the memory access application, “set” and “hold” conditions should be satisfied. The memory set condition is same as the switch condition that requires a desired transition among the states (blue and yellow arrows). The closed feedback loops for all three states with input intensity condition $T_2 < I_0 < T_3$ represent the memory hold condition (purple arrows).

The switching contrast in the extinction CS of the proposed resonator is provided in Table 5.3 for various switching (input) intensities identified with threshold levels in Figs. 5.6(b) and 5.7(b). These refer to corresponding switching between states depicted in the state flow diagram in Fig. 5.8(b).

For practical applications the plasmonic resonator must be cascaded with an external input intensity controller to provide switching and memory functionalities through self-modulation. An ideal candidate for this controller is a Vertical Cavity Surface Emitting Laser (VCSEL), whose output intensity is linearly proportional to the injected current under stimulated emission condition. The plasmonic
<table>
<thead>
<tr>
<th>Threshold Level</th>
<th>410 THz</th>
<th>498 THz</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Switching Intensity MW/cm²</td>
<td>Switching Contrast $</td>
</tr>
<tr>
<td>$T_1$</td>
<td>15</td>
<td>0.68</td>
</tr>
<tr>
<td>$T_2$</td>
<td>24.5</td>
<td>1.37</td>
</tr>
<tr>
<td>$T_3$</td>
<td>330</td>
<td>1.49</td>
</tr>
<tr>
<td>$T_4$</td>
<td>2123</td>
<td>0.34</td>
</tr>
<tr>
<td>$T_5$</td>
<td>5381</td>
<td>0.47</td>
</tr>
<tr>
<td>$T_6$</td>
<td>7114</td>
<td>0.30</td>
</tr>
</tbody>
</table>

Table 5.1: Switching power and contrast at various threshold switching levels [Figs. 5.6(b) and 5.7(b)].

resonator can be placed in the path of VCSEL’s output beam [Fig. 5.8(c)]. Finally, the schematic device model in Fig. 5.8(c) summarizes the proposed resonator’s use in optical communication and computing. The self-modulated input intensity $I_0$ controls the three-state resonator output “1/2/3”, which is compatible with 8B/6T “-/0/+” ternary line encoding schemes described in Fig. 5.1(a). It should also be emphasized here that the three-state switching capability is useful for communicating the multiplexed digital data that results from logic operations in computing devices sharing a common channel [Figs. 5.1(b) and 5.1(c)].

The portion of curves within the unstable regions are primary source of error for digital switching characteristics. During transients of the system, the output may reside in one of these unstable branches leading to ambiguity in the output state. However, once close to steady state the system will rapidly switch to one of its stable solutions. Also at high input intensity required for Kerr nonlinear operation the Joule heating may induce unwanted thermo-optic effects in the resonator. This may alter the predicted theoretical multi-stable response from the experimental case.

For certain applications switching response time should be known. Transient analysis can be done using time-domain simulators for this purpose. Several open-source finite-difference time-domain (FDTD) simulators can be used but they are
Figure 5.8: (a) Schematic of the proposed resonator’s tri-stable output. Stable branches are labeled as state 1, 2, and 3, within the tri-stability region. (b) State flow diagram of tri-stable system’s output. All transitions from one state to another are accompanied by the required changes in the input intensity level. (c) A schematic device model of the cascaded VCSEL controlling the input intensity of a nonlinear resonator with three-state output.
known to suffer from accuracy and stability problems especially for nonlinear and dispersive media for three dimensional models \[156\]. It was previously demonstrated that Kerr nonlinear response time of a thin-film Ag-BaO was 210 fs \[150\]. As the nanoscale localized surface plasmon resonances have low Q-factors, consequently it is expected that the switching times will be on the order of couple of picoseconds \[50, 143\]. It is estimated that with this time response the resulting switching operation will support a signal rate close to Tb/sec \[157\]. It should be also noted here that the maximum data rate is not only determined by the signal rate. The three-state output supported by the design increases the data rate by increasing number of digital symbols per signal from two to three, see 8B/6T scheme in Fig. 5.1(a).

Figures 5.6 and 5.7 clearly show that the input power required to generate bi- and tri-stability is rather high. The high power laser that has to be used for this purpose may cause several unexpected effects including localized thermal heating that may damage the metal patterns and $\chi^{(3)}$ material. The input power levels can in principle be reduced using a Kerr material with a higher $\chi^{(3)}$ coefficient. An example of such materials is organic polymer poly(β - pinene) Cu:Al$_2$O$_3$. Its nonlinear refractive index is on the order of 10$^{-14}$ m$^2$/W \[158, 159\] with $\chi^{(3)}$ coefficient which is on the order of 10$^{-17}$ m$^2$/V$^2$. These numbers imply that input power required to generate multi-stability effects can be reduced to MW/cm$^2$ level \[68, 71\].

Finally, a comparison of the proposed design to existing multi-stable output resonators is done from a practical implementation perspective: \[146, 147, 148, 149\]

(i) The thickness of the proposed device $t$ in the propagation direction is much smaller than those of band-gap structures and coupled resonators \[146, 147, 148, 149\]. This small thickness permits nanoscale integration of the device into an optical system and faster switching time.

(ii) Unlike band-gap structures \[146, 147, 148\] and coupled resonators \[149\] which work in a narrow band of frequencies, the proposed resonator has a broad band
of operation. The multi-stability is supported for visible and near infrared frequencies due to higher order plasmon modes generated on the resonator.

(iii) Compared to dielectric resonators [146, 147, 148, 149] the plasmonic resonator supports highly localized and strong near fields $|E_g|$ inside the gap allowing drastic enhancement of weak nonlinear $\chi^{(3)}$ process. Due to this enhancement the input intensity required for nonlinear operation is reduced.

5.4 Summary

A plasmonic resonator, which is capable of supporting multi-bi- and/or tri-stability in its response at the infrared and optical frequencies, is described. The capability to generate multi-level states can be envisioned as multi-state digital logic system that can operate beyond the traditional binary on-off switching. Applications for such three state optical switch is described for multi-level line coding and logic gates for time-division multiplexing schemes in digital communications. Such a device can be used in all-optical computing and communication applications.
Chapter 6

Concluding Remarks

6.1 Summary

In this thesis various types of plasmonic Fano nanostructures are proposed to manipulate light for sensing, electro-optical switching, near-perfect absorbing, and all-optical switching applications. More specifically,

(i) It has been demonstrated that the symmetry breaking mechanism could be used to generate two distinct Fano resonances in the visible spectrum. The scattering and absorption properties of these Fano resonances are found to be very sensitive to the surrounding medium. This implies that this kind of Fano resonators can be used to build devices capable of nanoscale optical sensing.

(ii) It has been demonstrated that a hybrid gold-graphene structure supports a Fano resonance at its out at THz frequencies. The spectral features of this polarization-independent Fano resonance are controlled by varying the gate voltage applied to the graphene patch. Slow light is also demonstrated inside the electromagnetically induced transparency window having a group index that exceeds 1500.

(iii) It has been demonstrated that the symmetry-breaking induced higher order surface plasmon modes on a multilayer graphene metasurface can be used to get
ultra broadband absorption. An unprecedented 50% increase in the normalized bandwidth is achieved over all the previously reported THz absorbers.

(iv) It has been demonstrated that exploitation of higher order plasmon modes equips a nonlinear resonator with a multi-band tri-stable response, which cannot be obtained using existing nonlinear plasmonic devices that make use of single mode Lorentzian resonances. Using self-tunable optical tri-stability, three-state all optical switching is realized using the proposed resonator having potential applications in optical communications and computing.

6.2 Future research work

Various research directions can be described based on the work proposed in this thesis. A few of them are listed below:

6.2.1 Acoustic Fano resonance

Research on electromagnetic Fano metamaterials can be extended to the acoustic regime. Designing an acoustic device, which supports a Fano-like resonance in its response to an incident sound wave, is indeed possible. The asymmetric Fano lineshape can originate from the interference of two longitudinal modes associated with two closely coupled resonators. Simultaneously, acoustically induced transparency (AIT) may also be achieved due to the destructive interference between the broad longitudinal resonance with the narrow band resonance. This kind of acoustic Fano resonators may be used to generate novel ultrasonic functionalities such as filters, collimators, and imaging via slow sound.
6.2.2 Polarization Independent Absorption

Symmetry breaking mechanism has proved to be useful for excitation of dark resonant plasmonic modes. However, it also leads to polarization dependent resonant absorption effects [64, 66]. Ideally such a metamaterial must be able to absorb light irrespective of incident polarization. This is only possible if the design of the metamaterial is polarization independent. For this purpose symmetric metasurface structures are being investigated for the excitation of higher order modes in order to achieve broadband absorption of THz-waves.

6.2.3 Enhancement of nonlinearity using plasmonic near-field

The Kerr nonlinearity enhancement using higher order modes on a plasmonic nanostructure is described for three-state switching in Chapter 5. Various other kinds of optical nonlinear processes (including second/third harmonic generation and four-wave mixing) can also benefit from the high near-field inside a plasmonic nanostructure. The higher order modes in plasmonic resonators can be used to extend the bandwidth of these nonlinear processes. The enhancement of these nonlinearities are beneficial for telecommunication and sensing applications.

6.2.4 Non-reciprocity of light

Non-reciprocal transmission of light can be used to build an optical diode (also known as isolator) that supports transmission of light in only one direction. Optical nonlinearity can be used to create a metamaterial device that supports non-reciprocal (asymmetric) transmission achieving high transmission contrast ratio. Cascaded nonlinear plasmonic resonators with broken symmetry in propagation direction can be exploited in order to achieve such asymmetric transmission to be potentially used as an optical diode.
6.2.5 Effective medium for describing asymmetric metamaterial response

The effective medium properties of an scattering object can be described by an equivalent homogeneous slab [123]. Characteristics of various kinds of electromagnetic metamaterials, which have been proven for negative index generation, cloaking and transformational optics, etc., have been analysed using effective medium models. If a given metamaterial exhibits a scattering response that is asymmetric (i.e., non-reciprocal), a scalar bilayer effective medium can also be used to represent its effective medium parameters.
REFERENCES


7 Papers Submitted and Under Preparation

Journals

Conferences
- M. Amin, M. Farhat, and H. Bagci. Dynamically-Tunable Graphene-Based Meta-

- Y. Khan, Y. Zhang, M. Amin, TK Ng, J. Philips, H. Bagci, B. Ooi, ZnO Nanorods for simultaneous light trapping and transparent electrode application in solar cell, *IEEE PS Annual Meeting* June 2011.