Terahertz metamaterial : surface lattice management with bound states in the continuum

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**NANYANG
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SINGAPORE

**TERAHERTZ METAMATERIAL: SURFACE LATTICE
MANAGEMENT WITH BOUND STATES IN THE
CONTINUUM**

THOMAS TAN CAIWEI

SCHOOL OF PHYSICAL AND MATHEMATICAL SCIENCES

2020

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MANAGEMENT WITH BOUND STATES IN THE
CONTINUUM**

THOMAS TAN CAIWEI

SCHOOL OF PHYSICAL AND MATHEMATICAL SCIENCES

A thesis submitted to the Nanyang Technological
University in partial fulfilment of the requirement for the
degree of Doctor of Philosophy

2020

The ouroboros...

Infinite cycle of life and unity of all

In loving memory of my grandfather...

Statement of Originality

I hereby certify that the work embodied in this thesis is the result of original research done by me except where otherwise stated in this thesis. The thesis work has not been submitted for a degree or professional qualification to any other university or institution. I declare that this thesis is written by myself and is free of plagiarism and of sufficient grammatical clarity to be examined. I confirm that the investigations were conducted in accord with the ethics policies and integrity standards of Nanyang Technological University and that the research data are presented honestly and without prejudice.

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Authorship Attribution Statement

This thesis contains material from 3 paper(s) published in the following peer-reviewed journal(s) / from papers accepted at conferences in which I am listed as an author.

Chapter 1 Section 1.3 is published as T.C. Tan, E. Plum and R. Singh. Surface Lattice Resonances in THz Metamaterials. *Photonics* **6(3)**, 75 (2019). DOI: 10.3390/photonics6030075.

The contributions of the co-authors are as follows:

- I prepared the manuscript drafts by collected the data from reference and input from all authors.
- Dr Eric Plum and Prof Ranjan Singh supervised and revised the manuscript.

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The contributions of the co-authors are as follows:

- Prof Ranjan Singh and Dr Manjappa provided the initial project direction.
- I wrote the drafts of the manuscript. The manuscript was revised together with all authors.
- Dr Srivastava prepared the samples and performed the spectroscopy measurements at the ultrafast terahertz photonics lab in Centre for Disruptive Photonic Technologies (CDPT) at School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore.
- I process and analyzed the data and prepared the figures with Dr Srivastava guidance.
- I coded and solved the coupled oscillator data.

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The contributions of the co-authors are as follows:

- Prof Ranjan Singh provided the initial project direction.
- I wrote the drafts of the manuscript. The manuscript was revised together with Dr Eric Plum and Prof Ranjan Singh.
- I designed the study and performed the spectroscopy measurements at the ultrafast terahertz photonics lab in Centre for Disruptive Photonic Technologies (CDPT) at School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore.
- I process and analyzed the data and prepared the figures.
- I performed all the simulations and designed the metamaterial structure.

Chapter 5 is in preparation for publication in *Advanced Materials* as T.C. Tan, Y.K. Srivastava, R.T. Ako, W. Wang, M. Bhaskaran, S. Sriram, I. Al-Naib, E. Plum and R. Singh, Nano-dielectric-induced active quasi-bound states in the continuum: A flexible metasurface platform for terahertz switching and sensing applications.

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- Dr Al-Naib provided the inspiration for the design.
- I wrote the drafts of the manuscript. The manuscript was revised together with all authors.
- R.T Ako, M. Bhaskaran and S. Sriram prepared the samples for Ge deposition in ARC Centre of Excellence for Transformative Meta-Optical Systems, RMIT University, Melbourne, Australia.
- Dr Srivastava and I did the Ge deposition in Centre for Disruptive Photonic Technologies (CDPT) at School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore.

- I designed the study and performed the spectroscopy measurements at the ultrafast terahertz photonics lab in Centre for Disruptive Photonic Technologies (CDPT) at School of Physical and Mathematical Sciences, Nanyang Technological University, Singapore.
- Dr E. Plum and I modelled the general asymmetry.
- I performed all the simulations with the help of Dr Srivastava.
- W. Wang did the topological charge and eigenmode simulations.

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ABSTRACT

This thesis will discuss and highlight the importance of the lattice mode in minimising the radiative losses and enhancing the quality factor in metamaterial resonances. The study of lattice modes has been done extensively in plasmonic arrays, and we would like to extend it into the field of terahertz metamaterials. It is particularly important to understand the role of lattices modes when they are coupled to the eigen-structural modes of the metamaterial systems that could be engineered to support, either uncoupled eigen-resonances or strongly coupled modes including Fano resonance at terahertz frequencies. Fano resonance is known for its asymmetric feature and high-quality factor that arises from breaking the symmetry of the constituent resonator in a unit cell. Subsequently, Fano resonance also known to be a consequence of a symmetry broken bound state in the continuum, which at low loss supports ultrahigh quality factors that are difficult to be measured.

The lattice modes that are inherent in periodic structures play a pivotal role in mediating the coupling between constituent resonators and can also be utilized to resonantly couple to metamaterial resonance for quality factor enhancement. This mediative coupling is observed in an avoided crossing and can be modelled as two or more coupled oscillators. Likewise, resonant coupling with metamaterial resonance enhances the resonant fields with the help of the trapped surface fields of the lattice mode. Lattice mode coupling to narrow split resonances and Fano resonance was demonstrated and we achieved enhancement of quality factor up an order of magnitude. This proves that radiative losses can be further minimized through optimization of the lattice modes but still is significantly insufficient to achieve an ultrahigh quality factor known to quasi-bound state in the continuum.

Quasi-bound state in the continuum known to be excited through structural symmetry breaking have piqued the interest of many, due to its ultrahigh quality factor resonant states. A new concept and model were developed to show that a subwavelength thin dielectric can be used to support and modulate such resonance in a symmetric and metallic split ring resonator. Additionally, we have shown that it could be used as an active ultrafast filter or a micro-fluidic sensor.

The lattice mode could also directly excite and support a resonant mode and such modes requiring phase matching conditions, e.g. spoof surface plasmons and guided-mode resonances. These modes are very narrow and can be exploited for low loss application. Therefore, we hope that the lattice mode can be used as an optimising strategy for minimising the radiative loss in metamaterials and that the new proposed device could be used to support an active high quality resonance on any existing symmetric and metallic metamaterial. The development of low-loss THz devices is beneficial for the support of upcoming and future communication devices and technologies.

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CHAPTER 1

Introduction

1.1 Metamaterials

Material development have always been an essential step in the evolution of technology. It is evident in the development of electronics in all our smart devices, memory storage, and wireless or wired data transfer rates, i.e. Internet of things (IoT). The working principles of electronics are due to the material's intrinsic properties, and there is a limit to the natural materials available for the development of these devices. However, novel processes and concepts have been put forward and discovered to increase the limited selection of materials nature have to offer. Such novel materials are 2-dimensional (2D) materials, e.g. graphene and transition metal dichalcogenide (TMD or TMDC), and topological material and concepts, e.g. topological insulators, and topological photonics. Material concepts are ideas that enable manmade materials to possess unique properties and characteristics that are not found in nature. Metamaterial is one such concept where it comprises of periodic subwavelength structures which interact with light homogenously to display unique interactions with light.

Metamaterials have been proven to be a useful platform for creating materials with unique optical properties. The first metamaterial demonstrated is its ability and flexibility to create its permittivity (ϵ) and permeability (μ). This ability allows the refractive index to be engineered, $n = \sqrt{\epsilon\mu}$, that is not obtainable through natural materials. Figure 1.1 shows an illustration of the categorisation of materials, including metamaterials, in a permittivity and permeability plot.

Figure 1.1: Permittivity ϵ and permeability μ plot to classify materials into four quadrant.

Region I consist of materials with both positive permittivity and permeability, which includes most dielectric materials. The next quadrant, Region II, consist of metals, ferroelectric materials and doped semiconductors with negative permittivity and positive permeability. Region III is a dead zone where no naturally occurring materials have the property of both negative permittivity and permeability. The last quadrant, Region IV, are ferrite materials with positive permittivity and negative permeability. However, metamaterials can fill the dead zone in Region III.

The investigation of both negative permittivity and permeability was first reported theoretically by V. G. Veselago in 1968^[1], a century later after J.C Maxwell's published his equations in 1865^[2].

$$\begin{aligned}
 \nabla \cdot \vec{E} &= \frac{\rho}{\epsilon} & \nabla \cdot \vec{B} &= 0 \\
 \nabla \times \vec{E} &= -\frac{\partial \vec{B}}{\partial t} & \nabla \times \vec{B} &= \mu_0 \vec{J} + \epsilon \mu_0 \frac{\partial \vec{B}}{\partial t}
 \end{aligned} \tag{1}$$

Including electromagnetism to wave propagation, where $\rho = 0$ and $\vec{J} = 0$, the plane wave equations for the electric and magnetic components are $\vec{E} = E_0 \exp(i\vec{k} \cdot \vec{r} - i\omega t)$ and $\vec{H} = H_0 \exp(i\vec{k} \cdot \vec{r} - i\omega t)$ respectively. Hence the curl equations simplify to $\vec{k} \times \vec{E} = \mu_0 \omega \vec{H}$ ($\vec{B} = \mu_0 \vec{H}$) and $\vec{k} \times \vec{H} = -\epsilon \omega \vec{E}$. These equations show the orthogonal relationship of the three vectors $(\vec{k}, \vec{E}, \vec{H})$ and if the wave propagates to a medium with $\epsilon > 0$ and $\mu > 0$, it will refract to the right obeying Snell's Law ($n_i \sin \theta_i = n_r \sin \theta_r$) as shown in the right of Figure 1.2. While for the left-hand propagation to occur and still satisfy Maxwell's equation, the material must be $n < 0$ ($\epsilon < 0$ and $\mu < 0$). This left-hand propagation material will be then made known as "left-handed" material (LHM) by Veselago.

Figure 1.2: Light refracting of two different mediums, left-handed material ($n < 0$) and right-handed material ($n > 0$), and obeying Maxwell's and Snell's equations.

Vesalago's theory was not realized until 1999 when Pendry et al. proposed a new category of materials which are metamaterials^[3]. It opened an entirely new field of research which is still relevant today. Though metamaterials are artificially created, it still obeys classical electromagnetics where the material properties with charged electric or magnetic oscillations are described by the Drude-Lorentz model given by:

$$\begin{aligned}\varepsilon_r(\omega) &= 1 - \frac{\omega_{p,e}^2}{\omega^2 - \omega_{0,e}^2 + i\gamma_e\omega} \\ \mu_r(\omega) &= 1 - \frac{\omega_{p,m}^2}{\omega^2 - \omega_{0,m}^2 + i\gamma_m\omega}\end{aligned}\tag{2}$$

where the subscript e and m refers to the electric and magnetic charges respectively, while ω_p is the plasma frequency, ω_0 is the resonant frequency and γ is the damping factor related to material losses. The ω_p of metals is at UV frequency and due to the free-electron approximation, $\omega_0 = 0$. Therefore, below the plasma frequency metals have real and negative permittivity, and all naturally occurring non-magnetic materials have $\mu_r = 1$. Because metamaterial consists of periodically arranged structures that are much smaller than the electromagnetic (EM) waves ($\ll \lambda$). The EM waves cannot sense the individual response of the structure, but collectively the metamaterial reacts with the EM waves homogenously with effective relative permittivity ($\varepsilon_{r,eff}$) and permeability ($\mu_{r,eff}$). Pendry's proposed structures for negative permittivity and permeability consists of wires and split-ring resonators (SRR) as shown in Figure 1.3. The wires have effective relative permittivity, effective plasma frequency and the damping factor as:

$$\begin{aligned}\varepsilon_{r,eff}(\omega) &= 1 - \frac{\omega_{p,eff}^2}{\omega(\omega + i\gamma)} \\ \omega_{p,eff}^2 &= \frac{e^2 n_{e,eff}}{\varepsilon_0 m_{e,eff}} = \frac{2\pi c^2}{d^2 \ln(d/r)} \\ \gamma_{eff} &= \frac{\varepsilon_0 d^2 \omega_p^2}{\pi r^2 \sigma} \approx 0.1 \omega_{p,eff}\end{aligned}\tag{3}$$

where σ is the conductivity of metal ($\sim 10^7$ S/M), the wire radius $r = 1$ μm , the lattice constant $d = 3.5$ mm. The results of the equations is an effective plasma frequency $\omega_{p,eff} = 7.52 \times 10^{10}$ rad/s, which is several orders smaller than metals. The effective relative permittivity is shown in Figure 1.3(b). The effective relative magnetic permeability of the SRR is:

$$\mu_{r,eff}(\omega) = 1 - \frac{F\omega^2}{\omega^2 - \omega_0^2 + i\Gamma\omega} \quad (4)$$

where the filling ratio $F = \pi r^2/d^2$ and the resonance frequency derived from the equivalent model $\omega_0 = \sqrt{\frac{1}{LC}} = \sqrt{\frac{3sc^2}{\pi^2 r^3}}$. L and C represents the geometric inductance and capacitance of the SRR. The lattice distance for the SRR is $d = 4$ mm, the spacing between the two concentric SRR is $s = 0.1$ mm, and the radius of the outer SRR is $r = 1$ mm. This parameter results in a resonance frequency of $f_0 = \omega_0/2\pi = 8.324$ GHz and at this frequency, the permeability is negative as shown in the permeability plot in Figure 1.3(d). Similarly, at this frequency, the permittivity of the wires is negative, and this is the strategy that Smith et al. took to demonstrate negative refraction at a single frequency experimentally. The metamaterial used by Smith et al.^[4-6] consists of a composite of both copper wires and SRRs metamaterial. Instead of a planar configuration, a 3-dimensional (3D) configuration is used, as shown in Figure 1.3(e).

Figure 1.3: Negative refraction metamaterial consisting of rods and split-ring resonators.^[5, 7] Adapted with permission from ref [5], Royal Society of Chemistry and [7], The American Association for the Advancement of Science.

For more complex structures, deriving the effective relative permittivity and permeability is very difficult. However numerical software such as COMSOL Multiphysics and CST Microwave Studio can calculate the transmission and reflection of complex metamaterials. The refractive index (n_{eff}) and the impedance (z_{eff}) can then be calculated using the transmission coefficient (t) and reflection coefficient (r) with the following equations^[8]:

$$n_{eff} = \frac{\pm 1}{k_0 L} \cos^{-1} \left(\frac{1 - r^2 + t^2}{2t} \right) + 2m\pi$$

$$z_{eff} = \pm \sqrt{\frac{(1 + r)^2 - t^2}{(1 - r)^2 - t^2}}$$
(5)

where the angular wavenumber in vacuum $k_0 = 2\pi/\lambda_0$, the thickness of the metamaterial L and m is an integer. In a passive medium, the real part of z_{eff} and the imaginary part of n_{eff}

should be positive. The permittivity and permeability can be calculated from the refractive index and impedance by $\epsilon_{r,eff} = n_{eff}^2 / z_{eff}^2$ and $\mu_{r,eff} = n_{eff}^2 \cdot z_{eff}$.^[9]

The introduction to negative refraction allows applications such as perfect lenses and invisibility cloaks which were not possible with conventional materials. Conventional lenses are limited by diffraction limits which perfect lenses are able to work beyond this limit. The concept of invisibility cloaks enables to hide the object the metamaterial is covering, as it bends the light around the object and allows the observer to see “through” the object.

1.2 Classification of Planar THz Resonator Resonances

Other than engineering the permittivity and permeability, metamaterial also has the flexibility to design resonances in the transmission or reflection spectrum. These resonances are obtained from either metallic or dielectric structures. This thesis will be focusing on resonances from metallic structures. The free electrons in metals, interact and couple to the incident light, oscillates and resonates. However, these oscillations are the majority cause of loss in metallic systems due to the ohmic losses from the resistance of free electrons scattering. This ohmic loss can be minimized with high conductivity metals, but it is still a substantial loss when compared to a well-designed dielectric resonator where quality factors could be an order magnitude higher than metals. One minor drawback in dielectrics is its structural dimensions, where it is resonant on the same scale as the wavelength instead of being subwavelength. The fabrication of dielectric is also much more demanding than metallic thermal evaporation.

The most common resonance is the dipole resonance which can be found in metallic structures, such as strips or any basic shaped resonators, as shown in Figure 1.4. In the Figure, the metamaterial is simulated with aluminium ($\sigma_{Al} = 3.56 \times 10^7$ S/m) on silicon substrate ($n_{Si} = 3.45$), simulation methods will be discussed in Chapter 2. The resonators are designed with a resonance at about 0.75 THz and have features that are broad and symmetric. The three

resonators shown have the same unit cell period, $P = 80 \mu\text{m}$, and the resonance is dependent on the geometry and substrate refractive index. Throughout this chapter, the scale of the surface currents is kept the same for comparison and the maximum current strength are displayed. The broad spectral lineshape is due to the highly radiative nature of the free electron oscillation. These oscillations are in phase and readily couples to the incident light (E_x or E_y), as seen in the parallel surface currents mimicking an electric dipole. In general, if the geometry of the metamaterial is symmetric about the x - and y -axis, the metamaterial will not be dependent on the polarization of the incident light.

Figure 1.4: Different metamaterial, (a) bar, (b) circle and (c) square resonator, with a dipole resonance at about 0.75 THz and its respective y -polarized surface currents. The square unit cell of each metamaterial is $P = 80 \mu\text{m}$ and the width is $6 \mu\text{m}$. The length of the bar, circle and square resonator is 70 , 65 and $55 \mu\text{m}$ respectively.

The ring-type resonator can be extended by introducing a gap, this induces a capacitance (C) and inductance (L), as mentioned by Pendry's first metamaterial. This LC-type resonator shown in Figure 1.5 with the (a) circle and (b) square-shaped resonator, forms a closed current-carrying loop from the capacitance gap which induces an inductance. This LC resonance f_1 , is less radiative and narrower than the dipole resonance as similar to electronics; the energy is stored in the capacitor and inductor. Because the structure is not symmetric about the x -axis, there is a polarization dependence between the resonances. Between the x and y polarization, there is an order-like behaviour between the resonances and it can be seen in the branches of the surface currents. In the x -polarization where the light is polarized along the gap, where previously would be degenerate to f_2 , splits into f_1 and f_3 . The LC-resonance f_1 is the fundamental resonance with a single closed loop surface currents, while f_3 is the third-order resonance with three branches of surface currents. The second-order f_2 can be seen in the y -polarization with the parallel surface currents as mentioned before as the dipole resonance.

Figure 1.5: LC-resonators, (a) circular and (b) square, with polarization dependant resonance and its respective resonance surface currents. Gap of 3 μm is introduced to the resonator.

The LC-resonator can be further extended by adding another gap symmetrically on the bottom. This additional gap breaks the single resonator in a unit cell to two constituent resonators which are also known as an SRR. If the SRR is independently symmetrical in x and y , the dipole mode is observable but at different frequency due to the gap, as seen in the black lines of Figure 1.6(b) and (c). If an asymmetry is introduced by shifting one or both of the gap, this changes the coupling between the two constituent resonators and results in a hybridized resonance where a split, EIT-type or Fano-type resonances can be observed. The coupling can also be physically quantified by an avoided crossing of resonances which signifies the strong coupling of the system. This system and a modified design will be thoroughly investigated together with the lattice mode in the following chapters.

Figure 1.6: Simulated transmission of an asymmetric split ring resonator. (a) Split ring resonator with two, 3 μm gap and polarization dependent resonance, (b) hybridized split resonances and (c) Fano-type resonance.

1.3 Surface Lattice Modes at THz Frequencies

Another phenomenon that is inherent in all metamaterials is the lattice mode, which arises from the collective diffractions from the periodic structures in the metamaterial array. It was first perceived as an optical anomaly by Robert W. Wood in his diffraction grating experiments^[10] in 1902. It opened two interesting research areas, categorized into *diffractive anomaly* and *diffusive anomaly*.

The diffractive anomaly refers to discontinuities in reflectivity measurements at unique combinations of illumination angle and wavelength, which were first observed by Robert W. Wood as resonant anomalies in grating structures^[10]. It was later interpreted by Lord Rayleigh to be a diffraction order and is referred to as Rayleigh anomaly described by a simple one-dimensional grating equation^[11, 12]:

$$\lambda_R = \frac{Pn_a}{i}(-\sin \theta_{\text{inc}} \pm 1), \text{ where } i = \pm 1, \pm 2, \dots \quad (6)$$

and λ_R is a Rayleigh wavelength, P is the grating period, n_a is the refractive index of the diffracting medium and θ_{inc} is the angle of incidence. This anomalous scattering allows the observation of extraordinary reflection, transmission, emission of light and near-field enhancement^[13-23].

The diffusive anomaly is closely linked to plasmonics and was explained by Ugo Fano in 1941 to be excitations of surface plasmon polaritons (SPPs) on a periodic metal-dielectric interface^[24]. This excitation arises from the coupling of electromagnetic waves to the oscillating electron plasma in conductors, which is evanescently confined at the metal and dielectric interface.

Another resonant phenomenon that has been studied extensively and arises from the electron plasma of conductors is the localized surface plasmon (LSP). It is specific to the scattering of subwavelength-size conductors and dependent on the geometry of the conducting

particle. The applications of LSPs include subwavelength imaging, sensing, lensing and lasing^[25-36].

While LSPs are dependent on geometry, SPP excitation requires momentum matching and the momentum of an SPP supported by a single continuous metal-dielectric interface is given by the SPP wave vector $\vec{k}_{sp}$ ^[37, 38]:

$$|\vec{k}_{sp}| = \frac{\omega}{c} \sqrt{\frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d}} \quad (7)$$

where ω is the SPP's angular frequency and c is the speed of light in vacuum, while ϵ_m and ϵ_d are the permittivity of the metal and dielectric, respectively.

Equation (7) can be extended to a perforated interface that is periodic in one (x , with $j = 0$) or two (x, y) dimensions. Since the surface waves are confined to planar interfaces, higher dimensions are not considered. Using Bloch wave momentum conservation from the grating coupler equation: $\vec{k}_{sp} = \vec{k}_{||} + i\vec{G}_x + j\vec{G}_y$, where $i, j = 0, \pm 1, \pm 2, \dots$ are the orders of periodicity, $k_{||} = k_0 \sin \theta_{inc}$ is the in-plane momentum of the incident light at the metal-dielectric interface, k_0 is the overall momentum of the incident light, while $\vec{G}_x = \frac{2\pi}{P_x} \hat{x}$ and $\vec{G}_y = \frac{2\pi}{P_y} \hat{y}$ are the reciprocal lattice vectors for the periods P_x and P_y along the unit vectors $\hat{x}$ and $\hat{y}$. At normal incidence $k_{||} = 0$ and the expression for the surface lattice resonance (SLR) frequency f_{SLR} can be defined to be^[39, 40]:

$$f_{SLR} = \frac{c}{\sqrt{\epsilon_e}} \sqrt{\frac{i^2}{P_x^2} + \frac{j^2}{P_y^2}} \quad (8)$$

where $\epsilon_e = \frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d}$ is the effective permittivity of the metal-dielectric interface and (i, j) are integer indices defining the SLR order along (x, y) . For an interface that is periodic in two dimensions (x, y) , i.e., a 2D grating, both indices can be non-zero. For a 1D grating, we have

$j = 0$, and the square root simplifies to i/P , and for a square lattice it simplifies to $\frac{1}{P} \sqrt{i^2 + j^2}$.

This expression can also be obtained from Equation (6) at normal incidence ($\theta_{\text{inc}} = 0$).

If the real part of the SPP in-plane eigenfrequency dispersion curves from Equation (7) is below the vacuum light line while the imaginary part is negligible, this indicates a bounded surface wave or guided-mode resonance. They manifest as a broad resonance peak or dip, while Rayleigh anomalies are observed as sharp peaks/kinks in the transmission spectrum^[41].

Surface waves can exist on periodic corrugated surfaces of any material. They are a result of diffraction of light from surface structures and also, in case of metals, of SPP excitation, where light couples to plasmons of the metal. Surface waves can be used to couple to metamaterial resonances, enabling various optical phenomena that are discussed below.

At terahertz frequencies, metals are very conductive and often taken to be perfect electric conductors ($|\epsilon_m| \gg |\epsilon_d|$), as their plasma frequencies are in the visible to ultraviolet part of the electromagnetic spectrum. Thus, the effective permittivity can be approximated as $\epsilon_e = \frac{\epsilon_m \epsilon_d}{\epsilon_m + \epsilon_d} \approx \frac{\epsilon_m \epsilon_d}{\epsilon_m} = \epsilon_d$ at terahertz frequencies^[42]. This approximation indicates that due to the high conductivity of metals at THz frequencies, the properties of SLRs only depend on the dielectric that forms an interface with the metal. This expression can also be extended to periodically arranged metallic metasurfaces, as one key feature that metasurfaces have in common with gratings is their periodicity. Therefore, the SLR expression was studied extensively in plasmonics^[43] and now could be extended to metasurface physics. SLRs could be used to couple with the eigen or coupled resonances of metamaterial structures to show fascinating effects. These effects include extraordinary transmission, reduction of radiative losses for high quality (Q) factor resonances, electromagnetically induced transparency and strong coupling physics between SLRs and metamaterial resonances^[44-52]. For a long time, the terahertz region of the electromagnetic spectrum was being referred to as the technological gap

between the infrared and microwave frequencies, which required more efficient and compact terahertz devices, sources and detectors^[53]. Now, the terahertz regime could potentially underpin the next generation of information and communication technology^[53, 54] as the communication carrier frequencies have been increasing continuously. Terahertz waves have also been proven to be beneficial in the medical and biological field as they are non-destructive and able to observe intermolecular vibrations that other frequency regimes cannot access^[55-59]. Another sector where terahertz waves have tremendous applications is that of homeland security. Due to the high conductivity of metals, metal detection imaging in airport security can be improved with THz technology, and due to the access to intermolecular vibrations, illegal drugs and explosives can be easily identified.

This section will cover the essential properties of SLRs, starting with the role of the lattice period, which not only determines the frequency of the SLRs but also coherent collective excitations in metamaterials. It will discuss how the coupling of SLRs to metamaterial resonances brings about Q -factor-enhancement, lattice-induced transparency, and lattice-mediated strong coupling in metamaterial systems.

1.3.1 Effects of Packing Densities in Metamaterials

The periodicity of metamaterials controls their SLRs; however, it also determines the packing density of resonators, which has additional effects on metamaterial properties. Periodically arranged subwavelength resonators collectively respond to incident light, but only a finite number of resonators is coupled in this collective resonant effect. The arrangement of resonators affects the resonance linewidth and depth as well as near-field subradiant coupling^[60-65]. Though the lattice period is used in investigating the metamaterial collective responses, the SLR is not required. To avoid SLR effects, J. Keller et al. used a silicon membrane instead of a thick silicon substrate to detune the SLR away from their metamaterial's

resonance at 1.12 THz^[64]. The metamaterial structure is a complementary split-ring resonator (SRR) or “Babinet structure”, consisting of an array of resonating apertures in a continuous copper film. Varying the lattice period between $P = 40$ and $180 \mu\text{m}$, they observed a resonance linewidth narrowing as the lattice period increased, as shown in Figure 1.7. Here, the resonance narrowing is not through resonant coupling to an SLR (which will be reviewed in the next section) but is due to the decrease of the meta-atom density as the resonator arrays become sparse. This linewidth (Δf) narrowing of resonance at the frequency f_0 can be quantified in terms of the Q -factor, $Q = f_0/\Delta f$, or the related decay rate is given by, $\Gamma = f_0\pi/Q$. A linear dependence of the decay rate Γ on the resonator density $\rho = 1/P^2$ and the square of the wavelength, λ^2 , was observed [Figure 1.7(c)]. This linear effect was interpreted as “Dicke superradiance” that arises from the coherent collective coupling of electric dipoles in the metamaterial system. A Lorentzian line shape is observed for the homogeneously broadening resonance when the resonators are densely packed. In contrast, Gaussian line shapes would be expected due to spectral broadening in inhomogeneous systems. A signature of superradiance in the linewidth broadening in metamaterials was also reported by R. Singh et al., where asymmetric line shapes of resonances were observed for larger lattice constants due to weak SLR coupling^[65]. Another study, by V. A. Fedotov et al., investigates the collective response of metamaterials as a function of the number of resonators and observes Q -factor-saturation at hundreds of metamolecules in a coherent metamaterial. This saturation indicates the number of resonators that can be coupled to determine the overall response of a coherent collective system and plays a role in engineering resonance characteristics, e.g., for lasing spasers^[60].

Figure 1.7: Split ring resonator (SRR) arrays with different packing densities. (a) Transmission amplitude of complementary SRR arrays for different lattice periods from, $P = 40$ to $180 \mu\text{m}$. Transmission for $P = 180 \mu\text{m}$ is multiplied by 10 to be visible on the same scale. (b) Normalized intensity transmission spectra for $P = 40, 100$ and $180 \mu\text{m}$ with their respective full width at half maximum. (c) The decay rate Γ as a function of the resonator density ρ multiplied by the square of the wavelength λ for the measured sample and simulations for three SRR geometries [see panel (d)]. Measurements are for a Si-membrane with Cu resonators, and simulations assume a conductivity of $2.5 \times 10^7 \text{ S/m}$ for copper or a perfect electric conductor (PEC) as indicated. (d) Simulated electric field enhancements for $P = 40 \mu\text{m}$ for the three SRR geometries.^[64] Adapted with permission from ref [64], John Wiley and Sons.

1.3.2 Q Factor Enhancement on Fundamental Resonances (Dipole and LC)

Metamaterial resonances are generally constrained by losses, which can be classified as radiative and non-radiative. Non-radiative losses are mainly due to the lossy nature of materials. Therefore, material selection plays an important role in reducing non-radiative losses and use of semiconductors, optimized resonator geometries, and gain media has been proposed to reduce or compensate such losses^[66-68]. Among metals, those with high conductivity, e.g.,

silver and gold, have low scattering rates of free electrons leading to low non-radiative losses, also known as resistive or ohmic losses^[67]. However, the oscillation of the free electrons couples easily to free space, causing metal structures to have significant radiative losses.^[69-71] When radiative losses dominate, their reduction will enable the metamaterial to trap energy for a longer duration, resulting in an improved quality factor of metamaterial resonances. Radiative losses can be reduced via smart array designs and, in this review, we will discuss how this can be achieved by resonant coupling of localized metamaterial responses with SLRs that are inherent to the periodic nature of metamaterials. Such coupling can be achieved by adjusting the SLR-wavelength (frequency) by varying the period P of the metamaterial array according to Equation (8), such that the SLR's spectral position becomes similar or identical to that of the metamaterial resonator's structural resonance, λ_{MM} .^[47] As shown by A. Bitzer et al. for the simplest case of normal incidence illumination of an array of point scatterers in a vacuum, when $P = \lambda_{MM}$, scattered field is trapped in the plane of the metamaterial array (lobes parallel to the y -axis of Figure 1.8). The trapped fields radiate along the plane of the array and can couple with localized metamaterial resonances, enhancing the localized fields within the metamaterial. This causes a reduction of radiative losses and can be observed as narrowed linewidth of the metamaterial resonances in the far-field. For example, this increases the resonance Q -factors of a simple split ring wire resonator supporting an inductive-capacitive (LC) mode and a quadrupole mode. Lattice mode coupling is very versatile and has been demonstrated on different types of metamaterial^[44-48, 50, 51] and plasmonic resonances^[25-27, 43, 52, 72-84]. This review highlights the SLR coupling to LC, dipole and hybridized modes of metamaterial resonators.

Figure 1.8: Scattering along periodic interfaces. The far-field intensity distribution of scattered light calculated for 1D arrays with different periodicities P_y located in the xy -plane and illuminated along z .^[47] Adapted with permission from ref [47], The Optical Society.

A simple metallic bar resonator oriented parallel to the incident polarization is able to support a dipole resonance mode characterized by charge oscillations, LSPs, along the bar. A simple split ring guides these charge oscillations along an inductive loop with a capacitive gap, as shown in Figure 1.9(a). N. Xu et al. demonstrated Q -factor-enhancement of normal modes of an SRR through coupling to a lattice mode by varying the lattice period.^[46] Resonator arrays with different periods excited by THz waves of appropriate polarization were used to couple a lattice mode to the metamaterial's LC mode ($n = 1$), dipole mode ($n = 2$) and quadrupole mode ($n = 3$). The LC and quadrupole modes are excited by incident light that is polarized perpendicular to the resonator's symmetry axis while the dipole mode is excited by light polarized parallel to the symmetry axis. Figure 1.9(b) shows the resonance line-narrowing and broadening of each mode as the lattice period increases from $P = 40 \mu\text{m}$ to $P = 200 \mu\text{m}$, where the narrowest linewidth occurs when the lattice mode matches the resonance frequency of the respective metamaterial mode. At these critical periods (P_{c1}, P_{c2}, P_{c3}), the Q -factor is maximized due to the reduction of loss in the system, as shown in Figure 1.9(c). This coupling enhances the Q -factor of the fundamental modes (LC and dipole mode) up to fifteen-fold and six-fold, respectively.

Figure 1.9: Enhancing split ring resonances using lattice modes. (a) Optical microscope images of the LC resonator metamaterial with its fixed resonator dimensions and at different period from 40 to 180 μm shown in the insets. (b) Simulated (i)–(iii) and measured (iv)–(vi) normalized transmission amplitude spectra showing different resonance modes ($n = 1, 2, 3$) for different periods. The resonant transmission minima were aligned to highlight the narrowing of the resonance linewidth. (c) Q-factor-enhancement in lattice-matched split-ring resonator arrays. Q-factor of the (i) LC ($n = 1$), (ii) dipole ($n = 2$) and (iii) quadrupole ($n = 3$) modes as a function of the lattice period. The polarization of the incident field is shown in the insets and the critical periods P_{cn} , where the lattice mode couples to the metamaterial resonance, are indicated by dashed lines.^[46] Adapted with permission from ref [46], AIP Publishing.

1.3.3 Lattice-Induced Transparency (LIT)

EIT is a phenomenon whereby an absorbing medium becomes transparent to a resonant probe beam under the influence of a stronger control or pump beam, resulting in a narrow transparency window. Within the transparency window, light experiences an anomalous phase change because of a steep dispersion. The induced steep dispersion of the medium can slow the propagation of light pulses by several orders of magnitude^[50, 85-87] and enhances nonlinear interactions^[88]. Such narrow and highly dispersive transparency windows possess a high Q -factor and are a promising platform for sensing and nonlinear applications. M. Manjappa et al. demonstrated a different phenomenon that introduces a sharp transmission peak by coupling the broad dipolar resonance of an asymmetric square resonator to the first order lattice mode as shown by Figure 1.10(a)^[44]. Previous understanding of metamaterial EIT is based on the near-field coupling of asymmetric metamaterial resonators: One so-called “bright” mode resonator will be coupled directly to the incident field and will have a broader resonance line width. A nearby so-called “dark” mode resonator is excited through near-field coupling from the “bright” mode resonator^[89, 90]. The bright mode is usually represented in the spectra as a bright dipolar resonance and the dark mode as an interference in the dipolar continuum resulting in a Fano resonance or EIT. This bright-dark mode coupling can be theoretically modelled as two coupled classical oscillators^[91]. Manjappa et al. observed that the lattice mode, in addition to the asymmetric dark mode, is also involved in inducing a narrow transparency peak termed lattice-induced transparency (LIT). The lattice mode can be modelled as another dark mode oscillator, as the energy diffracted from the incident field is being trapped within the near field of the metamaterial array and is not coupled to free space. Hence, the LIT system can be theoretically modelled using three coupled oscillators as seen in the inset of Figure 1.10(b), and the corresponding equations of motion are:

$$(-\omega^2 - i\omega\gamma_b + \omega_b^2)\tilde{x}_b + \Omega_1^2\tilde{x}_{LM} = \tilde{E}(\omega), \quad (9a)$$

$$(-\omega^2 - i\omega\gamma_{LM} + \omega_{LM}^2)\tilde{x}_{LM} + \Omega_1^2\tilde{x}_b - \Omega_2^2\tilde{x}_d = 0, \quad (9b)$$

$$(-\omega^2 - i\omega\gamma_d + \omega_d^2)\tilde{x}_d + \Omega_2^2\tilde{x}_{LM} = 0 \quad (9c)$$

where $(\tilde{x}_b, \tilde{x}_{LM}, \tilde{x}_d)$, $(\omega_b, \omega_{LM}, \omega_d)$ and $(\gamma_b, \gamma_{LM}, \gamma_d)$ are the amplitudes, angular resonance, and the damping frequencies of the bright, lattice, and dark modes, respectively. Ω_1 and Ω_2 are the bright-lattice and dark-lattice mode coupling strengths, respectively. In this model, the lattice mode is mediating the coupling between the bright mode and the asymmetric dark mode as expressed in Equation (9b). The lattice mode is an additional dark mode that induces strong near-field coupling between the bright dipole and the asymmetric dark mode, thereby enhancing the sharpness (Q -factor) of the induced transparency peak. Under resonant conditions, $\omega_d = \omega_{LM}$ and $\gamma_d = \gamma_{LM}$, the scattering amplitude of the bright eigenmode can be obtained from Equations (9a)–(9c). The transmission amplitudes in Figure 1.10(b) were obtained for realistic parameters of $\Omega_1 = \Omega_2 = 10^{12}$ (rad/s), $\omega_b = 6.9 \times 10^{12}$ (rad/s), $\gamma_b = 10^{12}$ (rad/s), $\gamma_{LM} = 0.15 \times 10^{12}$ (rad/s), $E = 0.17$ (V/m) and different lattice mode frequencies, ω_{LM} . As the SLR frequency is varied across the dipolar spectrum, the transparency peak is weakest at either side of the dipole spectrum and strongest when $\omega_{LM} \approx \omega_b$. The model does not include inter-unit cell coupling. These results demonstrate a unique phenomenon of inducing a narrow transparency peak, with Q -factors ranging from 25 to 91 extracted from Figure 1.10(a). This method also facilitates the frequency agility of the sharp transparency peak, which can be positioned precisely over a broad frequency range by choosing the lattice period. M. C. Schaafsma et al.^[50] reported lattice-enhanced transparency and slow-light effects in a periodic array of detuned dipole resonators. They considered metallic rods of two different sizes, in which the coupling of these metal rods with the lattice modes results in enhancement of the transmission window. Narrow transmission resonances mediated by the lattice may have

applications in the slow-light devices^[92-94] and as optical routers or light modulators for communication networks.

Figure 1.10: Lattice-induced transparency. (a) Transmission around a LIT resonance as a function of frequency and lattice constant for asymmetric split rings (inset)s. The red dashed-dot curve indicates the first order lattice mode $(0,1)$. (b) Transmission amplitude of the associated resonances extracted from the three-oscillator model of Equation (9) for varying lattice mode frequencies. For lattice modes in a silicon substrate, $\omega_{LM}/2\pi = 0.9, 1.084$ and 1.2 THz correspond to lattice periods of $P = 95, 80$ and $65 \mu\text{m}$, respectively. The schematic shows the underlying classical bright-dark-dark coupled oscillator model.^[44] Adapted with permission from ref [44], American Physical Society.

1.3.4 Lattice-Mediated Strong Coupling in Metamaterials

Due to the versatility and simplicity of the lattice mode. It can be coupled to many kinds of periodic systems, as discussed above. In case of LIT, a new mode or a split mode emerges when the SLR couples to the metamaterial and the coupling strength can be varied to observe different characteristic behaviours. If the splitting matches an avoidance crossing or anti-crossing eigensolution of a coupled oscillator mode and the coupling strength of the system is greater than the damping rate ($\Omega > \gamma$), the system is said to be strongly coupled. This can be achieved through coupling of a lattice mode to different metamaterial systems, directly, or indirectly, e.g., in case of LIT. Direct coupling of a lattice mode to a single-mode resonance resulting in splitting and anti-crossing was observed by A. Bitzer et al., see Figure 1.11. The

anti-crossing is between the (0,1) lattice mode and the split ring's $n = 3$ plasmonic structural resonance. The splitting occurs at point B in Figure 1.11(b), which marks the strong radiative coupling, as shown in [47].

Figure 1.11: Strong coupling between a single resonance and a lattice mode. Dispersion diagrams obtained from (a) measured and (b) simulated transmission spectra. The lattice constant, P_y varies from 380 to 1200 μm while P_x is kept constant at 380 μm . Plasmonic structural resonances are indicated by the grey dotted lines and the lattice modes by green and blue solid lines. A and B mark weak and strong radiative coupling for the $n = 3$ structural mode and a pure lattice mode is marked by C.^[47] Adapted with permission from ref [47], The Optical Society.

J. Keller et al. employ a complementary LC metamaterial resonator that supports a single, narrow resonance^[48]. Similarly, they observed a splitting in the LC resonance when it is coupled to the lattice mode. As their system is also strongly coupled, they were able to observe energy exchange between the modes in terms of resonance transmission amplitude at different lattice spacings, see Figure 1.12. An anti-crossing between the split LC mode and the SLR was also observed and modelled with a two-coupled oscillator model.

Figure 1.12: Lattice-induced resonance splitting. (a) Sample illumination for dipole mode (x-direction) and LC mode (y-direction) excitation. (b) Scanning electron micrograph of one split ring resonator with indicated dimensions. (c) (Left) Normalized transmission spectra of the measured (solid red lines) and simulated (blue dashed lines) metamaterial arrays at different lattice periods $P_x = P_y$. (Right) Simulated electric field distributions plotted in the y - z plane cut in the gap of the resonator. The field maps show the respective split modes for the lattice constants indicated on the right.^[48] Adapted with permission from ref [48], AIP Publishing.

1.4 Bound States in the Continuum

Recently, an extraordinary phenomenon called bound states in the continuum (BIC) have been growing in interest as they are bounded eigenmodes which exists above the photonic light line. This mode is a unique and a counterintuitive phenomenon as bounded eigenmodes are usually guided modes which are found below the light line. Physically BICs are localised mode within the radiation continuum, in which they are also known as embedded eigenvalues. These unique states were first theoretically predicted by von Neumann and Wigner in 1929.^[95] Theoretically, these BIC possess infinite lifetimes and zero linewidth which are very sensitive to any external perturbations.^[96, 97] Any slight perturbation could cause these bounded modes to be leaky. These leaky modes (quasi-BIC modes) will then have a finite lifetime and at low loss possess ultrahigh quality (Q) factors. At its lossy state, they are physically represented by a Fano resonance, and this link between Fano resonance and BIC were only discovered recently in metamaterials. Figure 1.13 illustrates different scenarios of possible BIC in (a) quantum wells and (b) photonics.^[98] In Figure 1.13(a), it illustrates two types of modes separated by a quantum well and its energy. Delocalized states that exists within the continuum and discrete bound states in the quantum well. While a BIC can be achieved by careful modulation of the quantum well potential energy. This concept which is extended to photonics to realize BIC with periodic waveguides as shown in Figure 1.13(b). In a simple waveguide, the modes fall below the light line, these are guided modes that do not leak to the far field. Structurally modulating the waveguide, there is a band folding due to the periodicity. This band folding allow for some modes to fall above the light line and the BIC emerges [circle in bottom panel of Figure 1.13(b)]. Figure 1.13(c) conceptualise the spectral profile of the BIC, resonance mode, the radiation continuum, and a regular bound state. While Figure 1.13(d) shows two cases of the quality factor of the resonance mode as it decouples of the radiation continuum. The first case demonstrates the quality factor of the resonance mode reaches infinity as a physical

parameter is adjusted to preserve symmetry; this is known as a symmetry-protected BIC. The second case, known as accidental BIC, maintains symmetry while tuning other physical parameters to achieve this decoupling of the radiation continuum.

Figure 1.13: Different concept of bound states in the continuum. Theoretical origin of BIC in quantum systems. (top) Conventional quantum well with the separation of localized and delocalized radiation. (bottom) Spatially modulated quantum well allows localization of a bound state within the continuous radiation. (b) BIC in photonic systems. (top) Guided mode falls below the light line, out of the radiative continuum, in a simple waveguide (bottom) Perforated waveguide, where band folding occurs from the periodicity and a BIC emerges (circle). (c) Conceptualizes states in a photonic system: Free space, regular bound states, extended state, resonance and BIC. (d) Different type of BICs in terms of Q factor, symmetry protected BIC and accidental BIC. (top) Q factor increases exponentially to infinity as BIC emerges from the preservation of symmetry. (bottom) Q factor approached infinity while tuning other parameters while preserving symmetry.^[98] Adapted with permission from ref [95], De Gruyter.

The most common type of BICs is the symmetry-protected BIC which will be the focus of this thesis. If a system possesses a mirror or 180° rotational symmetry (C_2), some resonant

modes are forbidden to radiate to the far-field. This symmetry protection can be seen in the disappearance and decoupling of photonic mode to the radiative continuum at $\mathbf{k}_{//} = (0,0)$, which is also known as the Γ -point. Away from the Γ -point, these modes start losing its symmetry protection and start to couple to the radiation in the form of resonance. Though the properties of BICs are very intriguing, it is challenging to observe and harness its infinite lifetimes in far-field experiments and applications. However, at its quasi-state, quasi-BICs possess very high-quality factors that are suitable for application such as lasing and sensing. Therefore, to access these high-quality states, the symmetry of the system must be disrupted. Other than varying $\mathbf{k}_{//}$ to break the symmetry, the angle of incident can be kept at the normal incident while changing the resonator's structural parameters. Figure 1.14 shows some examples of the symmetry breaking reported in metallic and dielectric metamaterials.^[99] It is also reported that the radiative quality factor follows a general law proportional to the inverse square of the defined asymmetric parameter.

Figure 1.14: Effects of in-plane asymmetry on the QBIC radiative Q factor. (a) Q factor dependence on in-plane asymmetry define by the meta-atom in (b). The decrease in Q factor follows an inverse square law of the asymmetry. (b) Different asymmetry meta-atom and the definition of asymmetry, α .^[99] Adapted with permission from ref [96], American Physical Society.

1.5 Active metamaterials

Active control in metamaterials plays a vital role in functionalising their engineered properties. In other words, if a metamaterial is engineered to be a narrow filter, active control would allow the filter to switch between bandpass and bandstop. Other active control function includes wave control, resonance modulation and switching and resonance frequency tuning. In this thesis, the focus will be on metallic structures; therefore, the discussion will be on the methods to actively change the response from metals. In metallic resonators, one method to add functionality is to incorporate active material with phase transitions where the optical response can be adjusted optically^[86, 94, 100-102], electrically^[102-104], or thermally^[105-107]. Figure 1.15 shows some active metamaterial design which is controlled by (a) electrical voltage^[104], (b) thermal^[105] and (c) optical^[100]. An example of phase transition would be semiconductors, an active dielectric, have adjustable-charge carriers to transition from an insulating state to a conducting state. Other active examples would include superconductors, phase change materials like GST, 2D materials like graphene, and semimetals. The capacitive coupling distance and the charge density of graphene enables resonance modulation. By gating the graphene as shown in Figure 1.1(a), the charge density can be increased through an external voltage bias which modulates and dampens the resonance. In Figure 1.15(b), a phase changing material, VO₂, is used as a square ring resonator on top of a split ring resonator and it changes from insulating at room temperatures to metallic at higher temperatures. At its metallic phase, the split ring resonators are shorted by the metallic VO₂, allowing asymmetric transmission followed by polarization modulation. Lastly, in Figure 1.15(c) shows optically controlled metamaterial device with the semiconductor, germanium. Through optical pumping, the germanium becomes more conductive and screens the whole device accompanied by the modulation of the resonator's resonance.

Figure 1.15: Different types of active metamaterial with (a) voltage, (b) thermal, and (c) optical control. (a) Schematic illustration of an SRR that is capacitively coupled to graphene electrodes and the transmittance modulation at various bias voltages.^[104] (b) Temperature controlled asymmetric transmission of vanadium dioxide sandwich in-between SRRs. The metamaterial transmits asymmetrically at low temperature (top) and symmetrically at high temperature (bottom) with the same linear polarization.^[105] (c) Optical images and the optical pumping schematic of the flexible metamaterial covered with Ge.^[100] Adapted with permission from ref [97] (American Association for the Advancement of Science), ref [101] (Springer Nature) and ref [102] (John Wiley and Sons).

Dielectrics are transparent in the terahertz region, and after pumping, they become more conductive. Therefore, the quick and easy strategy is to use dielectrics to change the metamaterial response by either altering the metamaterial structure or screening the whole metamaterial array. In split-ring resonators, the structural response can be altered by placing a dielectric patch in the gap to bridge and cause a short to the resonating arm, see Figure 1.16(a). At high conductivity, this dielectric patch changes the resonance from a split ring to a regular ring resonator. Figure 1.16(b) shows a similar outcome of resonance modulation, but instead of having the dielectric just in the gap, the dielectric in the same geometrical dimension of the SRR forms another layer underneath the SRR. While in the previous Figure 1.15(c), demonstrate resonance control by screening the whole metamaterial array with a germanium superstrate.

Figure 1.16: Types of optically controlled THz metamaterial. (a) Schematic of a coupled SRR-pair and a bar. A dielectric patch is placed in the gap of the SRR-pair.^[94] (b) Schematic of an asymmetric SRR with a dielectric resonator underneath with the same dimension as the SRR, without the gap. Optical modulation of the asymmetric SRR resonance.^[101] Adapted with permission from ref [91] (Springer Nature) and ref [98] (John Wiley and Sons).

1.6 Motivation of the Thesis

Earlier studies have shown that different metamaterial resonances can be coupled to achieve narrow resonant features mimicking electromagnetically induced transparency (EIT)^[89, 90, 108-110]. EIT type resonances in metamaterials involve near-field coupling between superradiant “bright modes” and subradiant “dark modes”. Bright modes are highly radiative and directly excited by the incident electric field, whereas dark modes arise from asymmetric near field coupling of the metamaterial elements, they are weakly coupled to the incident field and trap electromagnetic energy within the resonator^[92]. Similarly, metamaterial resonances could also be coupled to elementary excitations such as excitons^[111] or phonons^[112-114] to observe similar phenomena.

Since metamaterials are periodic structures with subwavelength lattice parameters, another class of dark modes exists in the array, the lattice modes. A lattice mode corresponds to diffraction along the interface of a periodic structure and mimics a surface plasmon polariton wave. In the metamaterial transmission and reflection spectra, the lattice modes are observed as kinks or discontinuities. The first order lattice mode (0,1) or (1,0) traps the diffracted field along the metal-dielectric interface of the periodic metamaterial array^[47]. Due to the trapped fields, the lattice mode behaves like a dark mode, and its resonant frequency can be easily controlled by changing the periodicity of the array. Coupling of the lattice mode to the eigenmodes of the metamaterial can lead to intriguing effects such as extraordinary transmission^[49, 115] and/or resonance linewidth narrowing^[47, 48] that give rise to extremely high quality (Q) factors. Control over Q -factor and depth of resonances have also been reported for three-dimensional metamaterials consisting of coupled resonators that can be tuned dynamically using MEMS approaches^[103, 116]. *The lattice modes that exist in any periodic array can be strongly coupled to allow linewidth and amplitude of resonances to be engineered while retaining the simplicity and low fabrication cost of planar metamaterials. High Q -factor*

devices minimize radiative losses and increase the sensitivity of the confined fields to external perturbations. These are characteristics needed in practical applications such as metamaterial spasers^[117], sensors^[118] and slow light devices^[50].

Controlling losses in metamaterials to obtain narrow resonances is important for photonic applications such as sensors^[119-121], low-power switches/modulators^[122], and narrowband filters^[53] across the electromagnetic spectrum. These losses can be non-radiative or radiative, and both can be minimised by choosing favourable materials and an optimal metamaterial design. Since Drude metals have high conductivity at terahertz frequencies, free electrons in the conduction band of metals experience little resistive heating when interacting with THz radiation, resulting in low non-radiative energy losses in non-resonant metallic structures. Therefore, radiative losses are the main cause of loss in non-resonant metallic THz metamaterials, where the oscillating fields of free electrons easily couple to free space. In symmetric structures, the incident field excites an in-phase collective dipole excitation of free electrons, which re-radiates efficiently to the far-field. However, a sharper resonance possessing a higher quality (Q) factor due to lower radiative losses can be realized by the destructive interference of different excitations. Such interference between a broad spectral line or continuum and a discrete resonance state gives rise to Fano^[123] resonances which are asymmetric in line shape. They were initially observed in quantum systems^[124-127] and the classical analogue of this phenomenon is also observed in a variety of photonic systems, including metamaterials.^[3, 128-131]

Recently, Fano resonances of metasurfaces have been linked to bound states in the continuum (BIC), which is a field of growing interest. BICs have bound eigenmodes which lie above the photonics light line^[96, 132-135] This itself is a unique counterintuitive characteristic and because of this, they possess infinite lifetimes and zero-linewidth resonances under ideal conditions.^[99, 136-138] *However, in the real world, ideal conditions are not possible, and*

therefore the investigation of a quasi-BIC (QBIC) is the only way to study BIC phenomena in the far-field. In this context, the QBIC is where the symmetry protected BIC collapses, resulting in loss of its infinite lifetime and zero linewidth. Hence the characteristics of QBIC include an extremely narrow linewidth which leads to an ultra-high Q factor. The small, but non-zero, losses of metals at THz frequencies prevent the realization of BIC and limit their QBIC approximations, but instead, Fano resonances can be observed easily. The link between the two, BIC and Fano resonance, is that both phenomena are a result of destructive interference coupling. *Therefore, methods that enhance Fano resonances to approach QBIC states with ultra-high Q factors could yield ultra-low-loss metallic metamaterial devices, as well as detectors with the resolution to pick up these narrow resonances.* ^[139]

One main concern is that BIC is limited to near-field measurements and to access these ultrahigh Q resonances requires low losses with asymmetry. While in metallic metamaterials, non-radiative losses still prevent the Q factor from matching that of dielectrics. One advantage metal has against dielectric is its subwavelength resonant nature; this allows the miniaturization of devices. The importance of miniaturization is seen in the electronics of our everyday devices such as smartphones, watches, tablets, and laptops. However, metallic metamaterial by itself does not provide functionality as their optical response are passive and not tunable. Consequently, hybrid metamaterial systems have been a strategy to incorporate the advantages of both subwavelength length scale metallic structure and tunable active control of dielectrics. Subwavelength metallic structures can be designed to support a broad range of resonances: dipole^[46], LC-type^[46, 140], Fano-type^[128-131, 141-143] and split resonances (includes EIT-type)^[45, 144-146]. The dielectric then supplements and functionalizes the metamaterial by enabling resonance switching and modulation. *However, it is not known that a subwavelength thin dielectric could support a QBIC resonance in a perfectly symmetric SRR on a low- n flexible substrate. This system is a general concept which could potentially be used with any dielectric*

on any symmetric platform for active control operations. Operations such as switching and modulation are required for active devices to control a signal or waveform. Miniaturization and speed are key in communications, where growing bandwidth requirements demand that we keep moving up in the frequency spectrum and the upcoming 6th generation (6G) telecommunications will fall in the terahertz regime.

1.7 Thesis organization

This thesis will cover the importance of surface lattice resonance coupling with metamaterials. SLR is studied extensively in plasmonic and can be extended to metamaterials. First, the SLR coupling is demonstrated in strongly coupled split-ring resonators in the form of an EIT-type or QBIC resonance. The coupling of SLRs to metamaterial resonances brings about Q -factor-enhancement, lattice-induced transparency, and lattice-mediated strong coupling in metamaterial systems. The SLR could be used as a strategy to further improve the Q -factor of high- Q Fano resonances to attempt to match that of QBICs. Next, the SLR is avoided with a low- n flexible substrate to prevent any diffractive loss to QBIC resonance. This low- n system is also designed to be a general concept for any thin subwavelength dielectric to support a QBIC resonance in a symmetric metamaterial array. Lastly, the thesis demonstrates the potential application to the nano-dielectric induced QBIC metamaterial.

In chapter 1, the discovery of metamaterials and split ring resonator's resonance was first introduced. Next, the effects and application of the surface lattice mode that is inherent in all metamaterial was discussed. Followed by general information of bound states in the continuum in metamaterials and lastly, the concepts of active metamaterials and their importance in applications.

In chapter 2, the simulation, fabrication and experimental methods are discussed. Simulations were done on a commercial software; CST Microwave Studio and the fabrication

process of a single step photolithography will be mentioned in this chapter. Spectroscopy measurements were done on a ZnTe terahertz time-domain setup that can be configured for optical-pump terahertz-probe (OTPP) spectroscopy or on a terahertz fiber system.

In chapter 3, the verification of lattice mode mediated strong coupling between the two hybridized metamaterial modes will be demonstrated. Resonance coupling between the SLR to each of the hybridized resonance resulting in enhanced Q factor was also observed. While a three-oscillator model is developed to verify the strong coupling of the system through an avoided crossing of resonances.

In chapter 4, a flipped split ring resonator was designed to flip the QBIC/Fano resonance closer to the surface lattice resonance which falls within the higher frequency spectrum. The electric and magnetic moment of the SRR was analysed and discovered that the lower frequency QBIC resonance arises from the electrical coupling while the higher frequency QBIC changes to a magnetic coupling in the flipped configuration. A resonance coupling between the SLR and QBIC was done to enhance the Q factor of the QBIC closer to the BIC state.

In chapter 5, a universal system for nano-dielectrics to support quasi-bound states in the continuum resonance on a symmetric metamaterial flexible platform was designed. The incorporation of the thin dielectric supports and actively controls the QBIC resonance through optical pumping. Subsequently, an ultrafast switchable filter and microchannel sensing were demonstrated. A universal model was developed to determine the Q factor and FoM through structural optimization of the nano-dielectric.

Lastly, in chapter 6 to conclude the thesis, a summary and closing statement of the thesis and the discussion of the possible future works on active guided mode resonance, BIC in non-symmetric systems and non-physical symmetry breaking of BIC.

1.8 Reference

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CHAPTER 2

Methodology

2.1 Simulation Methods

As mentioned in Chapter 1, where deriving the effective relative permittivity and permeability is difficult for complex structures. However, the effective relative permittivity and permeability can be calculated using the transmission and reflection coefficients obtained from numerical software such as COMSOL Multiphysics and CST Microwave Studio. Though calculating the effective relative permittivity and permeability is not required throughout the thesis, all the simulations for the transmission and reflection are obtained using CST Microwave Studios (CST). CST enables 3D modelling and electromagnetic response with transients or frequency domain solvers.

2.1.1 3D Modelling

In the modelling process, there are two steps to follow: (1) creating the model and material selection. (2) choosing the mesh and solvers. In Figure 2.1, CST provides a user-friendly interface that allows the creation of basic shapes such as (a) cuboid, sphere, cone, torus, and cylinder. For more complex shapes, CST also allows (b) line drawing and extrusion to convert the 2D line drawing to 3D. (c) Additionally, Boolean functions such as add, subtract, intersect, and insert can also assist in creating complex structures with cut outs or additional features. CST also includes transformation and symmetric functions such as (d) translation, scaling, rotation, and mirror to help assist in creating symmetric patterning of structures. During the creation of the 3D model, there is a choice for the type of material in the material library. The material will determine the dispersion type (metallic or dielectric), permittivity,

permeability, and conductivity. Other than using the build in properties, there are also user inputs for materials that are not found in the library.

Figure 2.1: CST Microwave Studio basic user operations for modelling. (a) 3D brick command for 3D structures with material input. (b) 2D drawings which can be also be extruded to 3D. (c) Boolean command for more complex structuring. (d) Transformation command.

2.1.2 Meshes and Solvers

After the modelling is to prepare the structure for solving and this is done by meshing. Meshing breaks down the structures in small hexahedral or tetrahedral elements. Below is the comparison of the two types of meshes.

Hexahedral mesh:

- Do not conform to interfaces of different materials.
- Compatible with Finite Integration Technique (FIT) or Transmission Line Matrix (TLM) types of solvers

Tetrahedral mesh:

- Conform to interfaces of different materials.

- Compatible with Finite Element Method (FEM) solver.

It is good practice to use both meshes for the same problems to compare and validate the results. Other software such as COMSOL can also provide the validations. The size of the elements is dependent on the features of the structures, the finer the mesh the higher resolution to pick up finer features like curves or thin structures. But a finer mesh would also mean longer computing time as there are more elements. Therefore, there must be a good balance between the size and number of elements. CST provide a pre-meshing before running the solver, this allows the troubleshooting for any mesh error (low quality elements) to be rectified by improving the element size. If the meshing includes low quality elements, the solver will miss out features that may be important in the EM interaction, hence affecting the results. Figure 2.2 shows an example of a LC ring resonator with a finer mesh than the substrate.

Figure 2.2: Meshing example and types of solvers. Top: Meshing and model example in CST Microwave Studio. Bottom: Time domain analysis and frequency domain analysis with respect to capability to simulate resonant device based on its quality factor.

After completing the meshing, the next step would be to choose the type of solver, frequency range and boundary conditions. There are two solvers that are used to obtain the metamaterial transmission and reflection, Time Domain and Frequency Domain solver. The time domain solver (Transient solver) is based on the FIT method which utilizes the discretized integral of Maxwell's equations and its solutions. While the frequency domain employs the Fourier transform of Maxwell's wave equations.

The bottom panel of Figure 2.2 shows the general purpose of each solver, if the simulation includes high quality resonant devices, frequency domain solver would be the better option. Since this thesis will be focusing on low loss high quality devices, the frequency domain analysis will be used.

Next initialization would be the frequency range and boundary conditions. The frequency range would be initialized to the bandwidth of the Terahertz Time-Domain Spectroscopy (THz-TDS), which will be discussed in the next section, of 0.2 – 1 THz. To resolve high-quality resonances in the simulation, for the bandwidth of 0.2 – 1 THz the initialization of the simulation resolution is set to 0.1 GHz (> 8000 points of simulation samples). Since the devices are metamaterials, the boundaries are periodic about xy -plane the boundaries in CST are initialized to “unit cell” option while in the z -axis is initialized to “open (add space)”. The model is now ready for simulation.

2.1.3 Simulations Results

The results $S_{z,\min}(1), S_{z,\max}(1)$, $S_{z,\max}(1), S_{z,\max}(1)$, $S_{z,\min}(2), S_{z,\max}(2)$ and $S_{z,\max}(2), S_{z,\max}(2)$ refers to the y -polarized (1) transmission (min, max) and reflection (max, max) and the x -polarized (2) transmission (min, max) and reflection (max, max), respectively. To isolate the metamaterial response from the substrate, the device transmission/reflection is normalized with the transmission/reflection of the substrate. This is also similar to the data processing done on the spectroscopy.

Other than obtaining the transmission and reflection, there are other simulation results such as electric or magnetic fields and the surface currents. This allow the visualization of the EM interactions such as field confinements, radiating fields and induced current in the metamaterials.

2.2 Coupled Oscillator Model

Resonances in metamaterial systems can be modelled with a theoretical classical model. A series of differential equation (equation of motion) can be used to describe the resonance frequency, damping rates, coupling strength and whether the system is driven with an external source. The quantities such as damping rate and coupling strength could determine if the system is strongly coupled to each other if the coupling strength is very much greater than the damping rate. This model can be used to describe the coupling interaction in a myriad of systems, such as coupling of primary excitations and cavity excitations.

2.2.1 Two Oscillator Model

The most fundamental coupled system is the two-oscillator model. This can be used to describe the coupling of a Fano system, where one of the oscillators is driven by the incident light and the other oscillator is driven indirectly through the coupling between the first oscillator. The direct driven oscillator is known as the “bright mode”, while the indirectly driven oscillator is known as the “dark mode”. In Fano system, this dark mode arises from the asymmetry of the system.

The equation of motion for the coupled two-oscillator model are,

$$\ddot{x}_b + \gamma_b \dot{x}_b + \omega_b^2 x_b + \Omega^2 x_d = E(t) \quad (10a)$$

$$\ddot{x}_d + \gamma_d \dot{x}_d + \omega_d^2 x_d + \Omega^2 x_b = 0 \quad (10b)$$

where, $x_{i=b,d} = \tilde{x}_i e^{-i\omega t}$, (ω_b, ω_d) and (γ_b, γ_d) are the displacement vectors, uncoupled resonance angular frequencies, and damping rates of the bright mode (b), and dark mode (d) respectively. Ω is the bright-dark mode coupling strengths and $E(t) = \tilde{E}(\omega) e^{-i\omega t}$ is the incident field, which directly couples to the metamaterial, resulting in a bright dipolar mode.

Solving the derivatives, transforms Equation (10) from the time domain to the frequency domain as shown below,

$$(-\omega^2 - i\omega\gamma_b + \omega_b^2)\tilde{x}_b + \Omega^2 \tilde{x}_d = \tilde{E}(\omega) \quad (11a)$$

$$(-\omega^2 - i\omega\gamma_d + \omega_d^2)\tilde{x}_d + \Omega^2 \tilde{x}_b = 0 \quad (11b)$$

The coupled equations can be solved with linear algebra by representing Equation (11) as a matrix,

$$\begin{pmatrix} \Lambda_b & \Omega^2 \\ \Omega^2 & \Lambda_d \end{pmatrix} \begin{pmatrix} \tilde{x}_b \\ \tilde{x}_d \end{pmatrix} = M \begin{pmatrix} \tilde{x}_b \\ \tilde{x}_d \end{pmatrix} = \begin{pmatrix} \tilde{E}(\omega) \\ 0 \end{pmatrix} \quad (12)$$

where $\Lambda_i = -\omega^2 - i\omega\gamma_i + \omega_i^2$ and $i = b, d$. The eigenvalues ω can be extracted by diagonalizing the matrix M by finding $\text{Det}(M) = 0$. The eigenvalues, ω , of the diagonalized matrix correspond to the two coupled modes of the coupled system.

2.2.2 Three Oscillator Model

To theoretically investigate the strong coupling between the resonator modes and the lattice mode in the next Chapter, we model the resonances with a three-oscillator model. This model was chosen to interpret both the simulations and experimental results. From previous studies, metamaterial EIT has been known to result from coupling between bright and dark modes^[1-5]. Coupling of our symmetric split-ring resonator with the lattice mode does not lead to any mode splitting, as the dark mode was not excited in this case. The observed dependence of EIT on the lattice period in this study indicates that coupling between the bright and dark modes may be mediated by the lattice mode (Figure 2.3). Therefore, we model the lattice mode as the mediator between the bright and dark mode, see Equation (13) below with the coupling strengths Ω_1 and Ω_2 .

Figure 2.3: Pictorial representation of the three-oscillator model, showing the coupling between the bright (b) and dark (d) modes with the lattice mode (LM) as the mediator.

The equations of motion for the three coupled oscillators are given as

$$\ddot{x}_b + \gamma_b \dot{x}_b + \omega_b^2 x_b + \Omega_1^2 x_{LM} = E(t) \quad (13a)$$

$$\ddot{x}_{LM} + \gamma_{LM} \dot{x}_{LM} + \omega_{LM}^2 x_{LM} + \Omega_1^2 x_b - \Omega_2^2 x_d = 0 \quad (13b)$$

$$\ddot{x}_d + \gamma_d \dot{x}_d + \omega_d^2 x_d + \Omega_2^2 x_{LM} = 0 \quad (13c)$$

where $x_{i=b,LM,d} = \tilde{x}_i e^{-i\omega t}$, $(\omega_b, \omega_{LM}, \omega_d)$ and $(\gamma_b, \gamma_{LM}, \gamma_d)$ are the displacement vectors, resonance angular frequencies, and damping rates of the bright mode (b), lattice mode (LM) and dark mode (d) respectively. Ω_1 and Ω_2 are the bright-lattice and dark-lattice mode coupling strengths, respectively. The incident field, $E(t) = \tilde{E}(\omega) e^{-i\omega t}$, directly couples to the metamaterial resonance, resulting in a bright dipolar mode. Whereas the dark mode arises from the structural asymmetric coupling and the lattice mode from the periodicity, and both do not directly couple to the incident field. Solving the derivatives of the displacement vectors and transforming Equation (13) from the time domain to Equation (14) in the frequency domain with the corresponding amplitudes $(\tilde{x}_b, \tilde{x}_{LM}, \tilde{x}_d, \tilde{E}(\omega))$ yields

$$(-\omega^2 - i\omega\gamma_b + \omega_b^2)\tilde{x}_b + \Omega_1^2 \tilde{x}_{LM} = \tilde{E}(\omega) \quad (14a)$$

$$(-\omega^2 - i\omega\gamma_{LM} + \omega_{LM}^2)\tilde{x}_{LM} + \Omega_1^2 \tilde{x}_b - \Omega_2^2 \tilde{x}_d = 0 \quad (14b)$$

$$(-\omega^2 - i\omega\gamma_d + \omega_d^2)\tilde{x}_d + \Omega_2^2 \tilde{x}_{LM} = 0 \quad (14c)$$

The parameters $(\omega_b, \omega_{LM}, \omega_d)$ and $(\gamma_b, \gamma_{LM}, \gamma_d)$ are taken from the experiments to match the model results. The bright mode frequency ω_b is the resonant frequency of the symmetric splitting resonator, whereas ω_{LM} and ω_d are obtained from the simplified expression of Equation (8) in Chapter 1 Section 1.3. ω_d is taken to be equal ω_{LM} as the lattice mode is assumed to mediate the coupling between dark to the bright mode. Based on the linewidths of the resonances, the damping rates were taken as $\gamma_b = 10^{12}$ rad/s and $\gamma_{LM} = \gamma_d = 0.15 \times 10^{12}$ rad/s while Ω_1 and Ω_2 are taken as free parameters for the numerical fitting (numeric

Matlab code can be found in the Annex) to solve Equation (14). The eigenvalues of the coupled equations can be solved by representing Equation (14) with a matrix as shown below

$$\begin{pmatrix} \Lambda_b & \Omega_1^2 & 0 \\ \Omega_1^2 & \Lambda_{LM} & -\Omega_2^2 \\ 0 & \Omega_2^2 & \Lambda_d \end{pmatrix} \begin{pmatrix} \tilde{x}_b \\ \tilde{x}_{LM} \\ \tilde{x}_d \end{pmatrix} = \begin{pmatrix} \tilde{E}(w) \\ 0 \\ 0 \end{pmatrix} \quad (15)$$

After that the eigenvalues are obtained from diagonalizing the matrix M by finding $Det(M) = 0$ and solving for ω .

$$M = \begin{pmatrix} \Lambda_b & \Omega_1^2 & 0 \\ \Omega_1^2 & \Lambda_{LM} & -\Omega_2^2 \\ 0 & \Omega_2^2 & \Lambda_d \end{pmatrix} \quad (16)$$

where $\Lambda_i = -\omega^2 - i\omega\gamma_i + \omega_i^2$ and $i = b, LM, d$. The eigenvalues, ω , of the diagonalized matrix correspond to the two hybrid modes of the coupled system and the lattice mode. A numerical fitting was performed to obtain the best values to fit the simulations. The coupling strength where $\Omega > \gamma$ tells us that the system is strongly coupled, which is physically represented by the anti-crossing.

2.3 Experimental Methods

2.3.1 Fabrication Methods

The general THz metamaterial fabrication follows a one-step photolithography process and thermal evaporation as illustrated in Figure 2.4. This is a general process done for metallic structures on high resistivity silicon. More details of the materials used will be described specifically in the respective chapter devices. First the silicon wafer is spin coated at 3000 rpm for 30 s with photoresist of 1.5 μm thickness. The wafer is then baked on a hot plate for 15 min at 115 $^\circ\text{C}$ to set the photoresist. After which the photomask containing the metamaterial structures are aligned on top of the coated wafer. This photomask allows the exposure of UV

rays to pass through the metamaterial patterns. The exposed area of the photoresist can be removed by the developing solution, this process is called the positive developing process. There is a negative process where the unexposed photoresist is removed, and this is mainly done for fabricating complementary metamaterial or Babinet structures. After removing the exposed photoresist, the wafer is being loaded into the vacuum chamber of the thermal evaporator. The thermal evaporator utilises high voltage to heat, melt and evaporate the metal to deposit to the wafer rotating above. The metal will be deposited to the exposed silicon and onto the photoresist. After depositing to the desired thickness, the wafer removed to be soaked in acetone. This is called the lift-off process where the metal on the photoresist will be removed leaving behind the metallic structures on the silicon.

Figure 2.4: Single step photolithography process with thermal evaporation of aluminium on a silicon wafer.

2.3.2 Terahertz Spectroscopy

All the metamaterial is characterized using Terahertz Time Domain Spectroscopy (THz-TDS). The illustration shown in Figure 2.5, shows the THz-TDS used for measuring the transmission of the metamaterial sample. The figure also shows the configuration for optical-pump terahertz probe (OPTH), where a second delay stage is used to control the optical path length of the optical pump beam. The whole THz path should be encased to allow the purging of air with nitrogen, this removes the moisture in air which is absorbent to THz.

Figure 2.5: Terahertz time domain spectroscopy and optical pump terahertz probe configurations. (1) Terahertz generation, (2) Terahertz detection and (3) Optical pump paths.

The setup uses a frequency down conversion sampling and a nonlinear generation of terahertz. The frequency down conversion requires a femtosecond pulse laser to sample the picosecond THz pulse. While the high-power pulse is required to generate THz from the nonlinear generation in the Zinc Telluride (ZnTe) crystal. The 800 nm laser pulse is generated from a Ti:Sapphire amplifier with a repetition rate of 1 kHz, a pulse-width of ~60 fs and power of ~6W.

If optical pumping is not required, only a single beamsplitter is used to split the beam to the (1) generation and (2) probe. The additional beamsplitter would split the beam to the (3) pump and to the first beamsplitter. The beamsplitter is an important component as it is the starting point for the optical path matching. For the pump beam the end of the optical path length is the sample and it should length should be equal to the length THz generation path from its beamsplitter. While for the generation beam, the end of the optical path is the detector and similarly should match with the THz generation from its beamsplitter.

In the generation path, lies the ZnTe THz emitter which convert the 800 nm pulses to THz through nonlinear optical rectification. The ZnTe crystal used for the generation is cut at $\langle 110 \rangle$, it is also non-centrosymmetric (no inversion symmetry) and large 2nd order nonlinear susceptibility ($\chi^{(2)} = 1.6 \times 10^{-7}$ m/V). Under strong optical field, the nonlinear optical phenomena consist of two prominent processes: second harmonic generation (SHG) and optical rectification. The bulk polarization induced by optical rectification is given by $P_0^{(2)} = 2\epsilon_0\chi^{(2)}(0, \omega, -\omega)|E_0|^2$, where $\chi^{(2)}(0, \omega, -\omega)$ is the second-order nonlinear optical susceptibility. This equation is the simplified version through solving the equations of motions for the nonlinear Lorentz model. Expanding the polarizability equation to $P = \chi^{(1)}E + \chi^{(2)}E^2 + \chi^{(3)}E^3 + \dots$. Given the applied electric field $E(t) = E_0e^{-at}$ propagating through the nonlinear crystal, a nonlinear polarization is induced by optical rectification is $P^{(2)}(t) =$

$P_0 e^{-2at^2}$. This time varying polarization in turn becomes a source for electromagnetic radiation, $P_0 e^{-2at^2} \propto |E(t)|^2$, generating THz. The upper limit of the spectral bandwidth of the newly generated radiation (THz) can be estimated to be the inverse of the optical pulse duration.

In the probe (detection) path, the variable delay stage allows the sampling of the THz pulse and the detection method is an electro-optic detection using a nonlinear crystal. The electro-optic effect is also known as the Pockels effect, where an electric field changes the birefringence of the medium (ZnTe). This birefringence would then change the polarization of the output beam, an illustration of the detection is shown in Figure 2.6 below.^[6, 7] In the case of the absence of terahertz field, the terahertz path is being blocked while the probe beam is able to pass through the detector. The probe beam will not experience the Pockels effect and change in polarization. The probe beam would then pass through the quarter waveplate, the Wollaston prism and lastly to the balanced photodetector. As the laser is linearly polarized, the quarter waveplate will be aligned to circularly polarized the beam. This circularly polarization would then split equally to the two orthogonally linear polarization through the Wollaston prism. The balance detector would do a difference detection between the intensities of the vertical and horizontal polarization (I_y, I_x). If polarization is completely circular, the vertical and horizontal components would be balance and zero. This will be the baseline and default configuration.

In the presence of the terahertz field, because of Pockels effect in the nonlinear crystal, ZnTe, the probe beam becomes slightly elliptically polarized. Passing through the quarter waveplate which was configured to circularly polarized a linear beam, tilts the elliptically polarized probe beam through a $\pi/2$ phase delay. Because of the elliptical polarization, there is an imbalance between the two orthogonally linear polarization as it passed through the Wollaston prism. This can then be detected by the balance detector due to the difference in the

imbalance in the intensities of the two orthogonal components. The stronger the terahertz electric field, the stronger the electro-optic effect, hence enabling the detection of the terahertz pulse.

Figure 2.6: Electro-optic detection of the terahertz pulse with the optical probe beam. Polarization dependence of the optical probe, without and with terahertz field.

In the THz-TDS, the acquisition of the transmitted time dependent electric field amplitude through the sample is $E_{sam}(t)$, as shown in the data processing example in Figure 2.7(a). In part (b) of the Figure, a Fast Fourier Transform (FFT) is done to transform the real-values time domain pulse into a complex-values frequency dependent THz electric field, $E_{sam}(\omega)$. The magnitude, $|E_{sam}(\omega)|$ is used for the data processing but other quantities such as amplitude and phase can as be extracted from the complex quantity. A normalisation

against a reference background is done by using Equation (17) to obtain the transmission spectrum, $T(\omega)$, as shown the Figure 2.7(c).

$$T(\omega) = \left| \frac{E_{Sam}(\omega)}{E_{Ref}(\omega)} \right| \quad (17)$$

The reference background could be air or the sample substrate, for a metamaterial sample. The data acquired from (a) and (b) would give the un-padded data in (c), it shows the finite resolution of the FFT resulting in a spectrum that is not smooth. The resolution of the FFT (ΔR_{FFT}) can be calculated with $\Delta R_{FFT} = 1/L_{pulse}$, where L_{pulse} is the time length of the time domain pulse. To smoothen and improve the resolution of the data as shown in the red spectrum of Figure 2.7(c), a processing method called zero-padding is performed to the time domain data before the FFT. Zero-padding increases the time length of the time domain pulse by adding zeros to the required length and FFT resolution. Though zero-padding can increase the number of frequency points with smaller intervals, it does not contain any additional information to alter the transmission response. In other words, to resolve narrower resonances, the physical scan length (un-padded length) in the time domain must be of the FFT resolution. Another information which can be obtain from the FFT result, is the bandwidth of the setup during an air scan. An example in Figure 2.7(b), the bandwidth is up to ~ 2 THz and beyond that the signal does not have sufficient strength to differentiate between the background noise as shown in Figure 2.7(c) at > 2 THz. Therefore, during the design phase, the structure is to be designed within the experimental bandwidth and resolution.

Figure 2.7: Terahertz spectroscopy. Measured (a) terahertz time domain pulse through a reference substrate and metamaterial sample, (b) FFT of the time domain pulse to frequency domain of the respective measurements in (a) and (c) transmission amplitude of the metamaterial normalised with the reference substrate.

The optical pump allows the measurements of transient dynamics of optically active materials. First the stage of the THz pulse through the photo-active sample is fixed at its maximum peak and the optical pump path is varied. Here, two process occurs, first is the photoexcitation and then the relaxation. These two processes are represented by the peak and fall of the $\Delta T/T_0$, where ΔT is the change in transmission due to the presence of the optical pump and T_0 is the absence of optical pump. At the peak of $\Delta T/T_0$, the optical pump pulse arrives at the same time as the THz pulse, as their path length are matched, and maximum photoexcitation occurs. After which the optical pulse is delayed from the THz pulse, which allows the excited material to relax back to its ground state. In the case for semiconductors

where the electrons can be optically excited, maximum photo-excited electrons occurs at the peak and as the pump pulse gets delayed, the electrons are able to relax back to the valance band. A multi-demodulator lock-in amplifier was used to measure both ΔT and T_0 to obtain $\Delta T/T_0$. A mono-exponential or higher order exponential fit can be used to extract the relaxation rate depending on the number of physical properties involved in the relaxation, e.g. electron-phonon, electron-exciton or trap assisted relaxation.

2.4 Reference

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CHAPTER 3

Lattice induced strong coupling and line narrowing of split resonances in metamaterials

3.1 Introduction

In this chapter, we investigate the coupling between the fundamental lattice mode and the hybridized resonances of a terahertz asymmetric split-ring resonator (TASR) metamaterial array with the incident electric field polarized parallel to the gap arm. We demonstrate Q -factor enhancement of an individual hybrid mode when it is resonantly coupled to the lattice mode and disappearance of the mode-splitting associated with decoupling of the lattice mode from the TASR eigenmodes. Hence, our results indicate that the mode splitting, also known as lattice induced transparency (LIT)^[1], requires coupling of the lattice mode to the TASR eigenmodes. These eigenmodes are the antisymmetric resonance mode that is excited due to structural symmetry breaking and the symmetric resonance mode that is a broad dipole resonance occurring in both perfectly symmetric as well as asymmetric structures. Through this lattice mode coupling and a three-oscillator model, we show the existence of an anti-crossing behaviour of the hybridized resonances that suggests a strong-coupling regime of the bright-lattice-dark (dipole-diffractive-asymmetric) mode interactions.

By varying the period P of the metamaterial unit cell, the frequency of the fundamental lattice mode can be tuned to couple to either of the two hybrid resonances. The frequencies of the lattice modes for a square lattice are given by

$$f_{LM} = \frac{c}{nP} \sqrt{i^2 + j^2} \quad (18)$$

where c is the speed of light in vacuum, n is the refractive index where the lattice mode propagates, P is the lattice period and (i, j) are non-negative integers defining the order of the

lattice mode. In our study, we only consider coupling between the metamaterial resonances and the first-order lattice mode (0,1) that propagates in the substrate of our metamaterial, for which $f_{LM} = c/nP$.

3.2 Method

Figure 3.1(a) shows the metamaterial array that consists of periodically arranged asymmetric split-ring resonators. The dimensions of the metamaterial's square unit cell are depicted in the inset of Figure 3.1(b). The asymmetry, $d = 8 \mu\text{m}$, is introduced in the structure by moving one gap away from the central vertical axis and the period P of the unit cell is varied to tune the frequency of the lattice mode. The metamaterial samples were fabricated using photolithography with positive photoresist (AZ5214E) on a double side polished, high resistivity ($> 5000 \Omega\text{-cm}$) silicon substrate of $500 \mu\text{m}$ thickness. A 200 nm thick aluminium layer was thermally evaporated over the patterned substrate and the undesired aluminium was lifted off using acetone. The fabricated metamaterial arrays have an overall size of $1 \text{ cm} \times 1 \text{ cm}$ each and an optical microscope image of a small portion of an array is shown in Figure 3.1(b). The samples were characterized using photoconductive-antenna-based terahertz time domain spectroscopy (THz TDS) and the transmission amplitude was obtained by normalizing $|t(\omega)| = |E_S(\omega)/E_R(\omega)|$, where $E_S(\omega)$ and $E_R(\omega)$ are Fourier transforms of the electric field transmitted through the metamaterial sample and a reference substrate, respectively. The metamaterial samples were loaded on a sample holder with a circular aperture of 10 mm diameter and characterized by a THz beam of 5 mm diameter, which corresponds to 25% of the exposed metamaterial area. Depending on the metamaterial periodicity, the illuminated area corresponds to 1400 to 4000 resonators.

Figure 3.1: Terahertz spectroscopy on an asymmetric metamaterial. (a) Schematic illustration of the TASR metamaterial array, which is illuminated by a THz beam of 5 mm diameter. (b) Optical microscope image of the fabricated metamaterial array, with its unit cell dimensions shown in the inset. P is the periodicity of the unit cell which is a variable parameter in this investigation. All unit cell dimensions are given in micrometers.

3.3 Lattice Mode Coupling to Hybridized Split Modes

First, numerical investigations were performed using the CST Microwave Studio Frequency Domain Solver to understand the effect of the periodicity variation on the resonances of the TASR metamaterial. The aluminum split rings were modelled with a DC conductivity of 3.56×10^7 S/m and the silicon substrate with a refractive index of $n = 3.42$. In the simulation, the periodicity P of the structure was varied from 70 μm to 120 μm to investigate the interaction of the first order lattice mode with the hybridized modes of the TASR. Figure 3.2 shows both simulated and measured transmission spectra, which are in good qualitative agreement. Quantitative deviations in the line-widths and amplitude of the resonances between the simulated and experimental results are mainly due to the low spectral resolution of the THz TDS setup. Deviations in the resonance frequencies of few percent are mainly due to fabrication imperfections. By increasing the period P from 70 μm to 120 μm , the spectral position of the first order lattice mode is varied to couple to the metamaterial

resonances. Through this coupling, the split-ring resonances redshift, and their spectral linewidth changes. Mode splitting (mode hybridization) with an intermediate transmission peak is observed. The resonant transmission amplitude minima and maxima of the metamaterial are narrowest at critical periods, where the lattice mode resonantly couples with either of the hybrid modes [Figure 3.2(b) and (f)] or the transmission peak [Figure 3.2(c)]. As the unit cell periodicity is increased above $90\text{ }\mu\text{m}$, the mode-splitting disappears [Figure 3.2(g) and (h)]. This indicates that coupling of the lattice mode to the metamaterial resonances in the TASR contributes to the hybridization of modes, which we address as the low frequency hybrid mode (LFHM) and the high frequency hybrid mode (HFHM). We note that the (1,1) order lattice mode can be seen for periodicities of $90\text{ }\mu\text{m}$ and $120\text{ }\mu\text{m}$ at frequencies of 1.38 THz and 1.03 THz, respectively [Figure 3.2(g) and 2(h)].

Figure 3.2: (a)-(h) Experimental (black spheres) and simulated (red solid lines) transmission amplitude of the TASR metamaterial array with varying lattice period $P = 70, 75, 80, 82, 84, 87, 90$ and $120 \mu\text{m}$, respectively. The low frequency hybrid mode (LFHM) and high frequency hybrid mode (HFHM) are indicated in (a) and arise from the lattice induced transparency (LIT). The fundamental lattice mode (0,1) is indicated by a dark blue triangle and the (1,1) order lattice mode is indicated by a green triangle.

3.4 Q Factor and Figure of Merit

As the lattice mode is swept across the metamaterial resonances, drastic changes occur in the linewidths and the resonance intensity of the LFHM, the HFHM and the LIT transmission peak in between. Figure 3.3 shows the Q -factor ($Q = f_0/\Delta f$) of the HFHM and the LFHM as a function of the lattice period, which is calculated from the transmission intensity $|t(\omega)|^2$, where f_0 is the resonance frequency and Δf is the line width measured as full width at half maximum (FWHM) of the resonance in the transmission intensity spectrum. As the lattice mode is swept across the HFHM resonance by increasing the lattice period from 65 μm to 82 μm , the Q -factor of the HFHM decreases gradually from 31 to 6, see Figure 3.3(a). As the lattice mode frequency falls below the HFHM, the HFHM resonance broadens and the associated transmission increases. The slight increase in Q -factor above the lattice period 82 μm is due to the increase in its associated transmission and the decrease of the transparency peak. This causes the baseline of how the intensity is calculated and its associated FWHM to decrease slightly. The resonant change in transmission becomes small at larger periodicities, see Figure 3.2. This could be due to decoupling from the lattice mode and a weaker collective response from the larger unit cells in the metamaterial structure^[2, 3]. On the other hand, as the lattice period is increased such that the lattice mode frequency approaches the LFHM, there is an exponential increase in its Q -factor, as shown in Figure 3.3(b). This exponential increase is due to the gradual increase in coupling of the lattice mode to the LFHM that confines the electromagnetic energy in the metamaterial array. At $P = 87 \mu\text{m}$, where the lattice mode resonantly couples with the LFHM, the Q -factor reaches 113 which is an order of magnitude higher than the HFHM of the same structure. In this case, both narrowing and reduced depth of the transmission resonance contribute to the observed exponential increase in the Q -factor. The practical importance of tailoring the Q -factors is apparent in terms of a figure of merit

(FoM), which also considers the strength of the resonance and is useful for designing efficient sensors and nonlinear devices. The figure of merit ($FoM = Q \times \Delta I$) is defined as the product of Q -factor and change in transmission intensity ΔI (depth) of the resonance spectra. Figure 3.3(c) and (d) show the FoM for the HFHM and LFHM resonances, which reach maxima of 11 and 19, respectively. Like its Q -factor, the FoM of the HFHM is largest at smaller periods. As the period increases from $65 \mu\text{m}$ to $87 \mu\text{m}$, it drops by an order of magnitude due to the broadening of the resonance, the increase in resonant transmission intensity and the vanishing of the neighboring LIT transmission peak at larger lattice periods. In the case of the LFHM, not only the Q -factor but also the FoM shows an exponential increase, which reaches a maximum FoM of 19 and Q -factor of 113 at $P = 87 \mu\text{m}$. At this period, the LFHM provides higher sensitivity and lower radiative losses due to the strong coupling with the lattice mode that enhances the confined near field energy in the split-ring gap.

Figure 3.3: Q -Factor and figure of merit (FoM) of the HFHM and LFHM of the asymmetric metamaterial for different periodicities: (a, b) Q -factors of the HFHM and LFHM reaching a maximum of 31 and 113, respectively. (c, d) FoM of the HFHM and LFHM reaching a maximum of 11 and 19 respectively.

3.5 Lattice Mode Electric Field Enhancement

Further investigation of the electric field confinement and surface currents of the lattice matched hybrid modes ($P = 75$ and $87 \mu\text{m}$) is shown in Figure 3.4. Little electric field confinement was seen in both hybrid modes at $P = 75 \mu\text{m}$ as the surface currents remain in a dipole configuration which is highly radiative. However, at $P = 87 \mu\text{m}$, when the lattice mode frequency closely matches the LFHM, the surface currents are in a quadrupole configuration resulting in strong electric field confinement and a high Q -factor of 113 [Figure 3.4(b), $P = 87 \mu\text{m}$, left]. Another point to note is that as the first order lattice mode crosses the LFHM, the surface currents and field distribution of the HFHM show a dipole configuration [Figure 3.4(b), $P = 87 \mu\text{m}$, right], which corresponds to a broad minimum in transmission. Interestingly, for periods larger than $87 \mu\text{m}$, the mode-splitting is barely visible in the spectrum (Figure 3.2), suggesting that the fundamental lattice mode decouples from the TASR eigenmodes and mode-splitting switches off. This investigation indicates the role of the first order lattice mode in the mode-splitting effect in the system. However, our structure also possesses a structural asymmetry that contributes to the observed mode-splitting. Therefore, a similar investigation was performed with a symmetric resonator (symmetric gap, $d = 0$) of otherwise same dimensions. No mode splitting was observed in the symmetric structure even under lattice matched conditions, as shown in Figure 3.5. Hence, our results show that the mode-splitting effect occurs under two conditions. First, the metamaterial resonator must be asymmetric, and second, the fundamental lattice mode must be close to the structural resonance of the metamaterial resonator.

Figure 3.4: Distributions of (a) electric field magnitude and (b) surface currents of the LFHM and HFHM for metamaterial periods of 75 and 87 μm . For $P = 75 \mu\text{m}$ the lattice mode is close to the HFHM and for $P = 87 \mu\text{m}$ the lattice mode is close to the LFHM. The LFHM for period 87 μm is a quadrupole mode with high field enhancement while the others are electric dipole modes.

Figure 3.5: Transmission amplitude of the symmetric metamaterial array (same unit cell dimensions in **Figure 3.1** of the main manuscript but with asymmetry $d = 0 \mu\text{m}$) for lattice parameters P of 70, 80, 90, and 110 μm . (a) Simulated and (b) experimental transmission spectra, with the arrow heads denoting the first order lattice mode.

3.6 Lattice Mode Mediated Strong Coupling

As the lattice mode is swept across the hybrid modes, not only the amplitude and width but also the spectral position of the resonance changes. The observed periodicity-dependence of the two hybrid mode frequencies reveals an anti-crossing behaviour, which is a signature of a strongly coupled system. We modelled this coupling with a three-oscillator model^[1, 4-6], which was described in detail in Chapter 2 Section 2.2.2. Its oscillators correspond to the symmetric bright mode, the lattice mode and the asymmetric dark mode which arises due to

the structural symmetry breaking. The coupled equations representing the interaction between the bright, lattice and dark modes are expressed as

$$(-\omega^2 - i\omega\gamma_b + \omega_b^2)\tilde{x}_b + \Omega_1^2\tilde{x}_{LM} = \tilde{E}(\omega) \quad (19a)$$

$$(-\omega^2 - i\omega\gamma_{LM} + \omega_{LM}^2)\tilde{x}_{LM} + \Omega_1^2\tilde{x}_b - \Omega_2^2\tilde{x}_d = 0 \quad (19b)$$

$$(-\omega^2 - i\omega\gamma_d + \omega_d^2)\tilde{x}_d + \Omega_2^2\tilde{x}_{LM} = 0 \quad (19c)$$

where $(\tilde{x}_b, \tilde{x}_{LM}, \tilde{x}_d)$, $(\omega_b, \omega_{LM}, \omega_d)$ and $(\gamma_b, \gamma_{LM}, \gamma_d)$ are the displacement amplitudes, resonance angular frequencies, and damping rates of the bright mode, lattice mode and dark mode respectively. Ω_1 and Ω_2 are the bright-lattice and dark-lattice mode coupling strengths, respectively. In this model, the lattice mode mediates the coupling between the bright and dark modes. Equation (19a) is the equation of motion for the bright mode and it is driven by the incident light, while (19c) is the equation of motion of the dark mode of the TASR, and they are both coupled to the lattice equation of motion (19b) by the coupling strengths Ω_1 and Ω_2 respectively.

The bright mode frequency of 1.1 THz is taken as the dipole frequency of a symmetric split-ring resonator, whereas ω_{LM} is obtained from the simplified expression of Equation (18). Also ω_d is taken to be equal to ω_{LM} as the lattice mode mediates the coupling of the dark mode to the bright mode in our model. Based on the linewidths, the damping rates were taken as $\gamma_b = 10^{12}$ rad/s and $\gamma_{LM} = \gamma_d = 0.15 \times 10^{12}$ rad/s while Ω_1 and Ω_2 are taken as free parameters. With this model, the eigenvalues of the coupled equations are solved through the diagonalization of matrix M:

$$M = \begin{pmatrix} \Lambda_b & \Omega_1^2 & 0 \\ \Omega_1^2 & \Lambda_{LM} & -\Omega_2^2 \\ 0 & \Omega_2^2 & \Lambda_d \end{pmatrix} \quad (20)$$

where $\Lambda_i = -\omega^2 - i\omega\gamma_i + \omega_i^2$ and $i = b, LM, d$. The eigenvalues of the diagonalized matrix are the two hybrid modes of the coupled system and the lattice mode. A numerical fitting was performed to obtain the best values to fit the simulations, resulting in $\Omega_1 = 2.30 \times 10^{12}$ rad/s and $\Omega_2 = 1.84 \times 10^{12}$ rad/s. As illustrated in Figure 3.6, the three-oscillator model (red circles) fits the simulations (green squares) well at larger periodicities. But the oscillator model does not account for the nearest neighbour coupling of the metamaterial unit cells, resulting in deviations at smaller periodicities, where the simulated resonance shift of the HFHM is less prominent than predicted by the analytical model. Figure 3.6 also shows the crossing of the period-dependent lattice mode and the bright dipole mode at 1.1 THz. This crossing corresponds to the high- Q lattice induced transparency peak shown in Figure 3.2(c). In this system, the lattice mode mediates the coupling of the bright mode to the dark mode, giving rise to the observed anti-crossing. Therefore, this anti-crossing behaviour alongside the coupling strength where $\Omega > \gamma$ is a signature of a strongly coupled system that can only be observed at periodicities $P < 90 \mu\text{m}$ as the mode-splitting vanishes at larger periodicities.

Figure 3.6: Resonance frequency of hybrid modes (LFHM and HFHM) and lattice mode with varying period of the metamaterial array according to simulations and analytical model. Anti-crossing behaviour is seen at the intersection of the Dipole mode of 1.1 THz (cyan dash) and the calculated lattice mode according to Equation (18) (blue dash). The green squares represent the two-hybrid split-ring modes from the simulation. The red circles represent the analytical eigensolution of the three-oscillator model.

3.7 Conclusion

In summary, we demonstrated how lattice modes can be used to control the strength and width of hybridized resonances in metamaterial arrays of asymmetric resonators. By varying the metamaterial periodicity, we selectively coupled the fundamental lattice mode to either of the hybridized modes of terahertz asymmetric split-ring resonators and were able to tune the resonance Q -factor of one hybrid mode from 5 to 113. We have also reported evidence of strong coupling between the bright, lattice and dark modes in the form of an anti-crossing behaviour using a three-oscillator model. This simple approach of in-plane coupling of the fundamental lattice mode and metamaterial resonances can be used as an efficient technique to optimize metamaterial designs to reduce radiative losses and to provide high- Q resonances for practical applications such as ultrasensitive sensors and low threshold lasing spasers.

3.8 Reference

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CHAPTER 4

Lattice enhanced Fano resonances from bound states in the continuum metasurfaces

4.1 Introduction

In this chapter, we experimentally study the coupling of the Fano resonance of an asymmetric split ring resonator (ASRR) to the first order lattice mode (FOLM) of the resonator array. Previous studies have shown enhanced Q factors by coupling a lattice mode to inductive-capacitive (LC) resonances^[1-3] and electromagnetically-induced-transparency-type (EIT-type)^[2, 4-8] resonances. Here, we demonstrate FOLM coupling to a Fano resonance obtained through magnetic coupling and observed both Q factor and FoM enhancement. The ASRR was designed to support a Fano resonance at about 1 THz and a dipole resonance at a lower frequency of 0.853 THz. Compared to a conventional square ASRR consisting of two end-coupled resonator arms, this was achieved by *flipping* the resonator arms resulting in an ASRR consisting of side-coupled resonator arms. The coupling nature of the ASRR is determined by analysing the electric and magnetic dipole moments of the transversely coupled resonator arms, which determines the symmetric and antisymmetric coupled modes represented by the higher and lower frequency split modes.^[9] Lattice mode coupling is achieved by tuning the lattice mode frequency f_{LM} . At normal incidence, $f_{LM} = \frac{c}{nP} \sqrt{i^2 + j^2}$ [Equation (18)], where c is the speed of light in vacuum, n is the refractive index of the medium where the lattice mode propagates, P is the periodicity of the square lattice and (i, j) are indices defining the order of the lattice mode. For this investigation, the first order lattice mode (FOLM) (0,1) – that propagates in the metamaterial’s silicon substrate – is used to interact with the metamaterial resonances. In the frequency ranges considered here, the metamaterials do not diffract in air. As the FOLM traps most of the THz energy on the surface of the metamaterial array, it

strengthens the resonant near-field confinement of the metamaterial resonance.^[10, 11] After the investigation of lattice coupling, angle-dependent simulations were performed on a symmetric resonator under ideal conditions to determine the nature of the Fano resonance. Our findings demonstrate the evolution of a BIC to a Fano resonance. Since an ideal BIC cannot be realized, one way of observing this phenomenon experimentally at normal incidence is to induce a QBIC through symmetry breaking of the resonators, which is well-known to lead to Fano resonances. An ideal BIC, characterized by infinite lifetime (infinite Q factor), is divergent in nature, however, it decreases to a finite quantity in response to any perturbation that breaks the in-plane symmetry, i.e. any illumination angle^[12] or structural parameter that makes the excitation of one resonator arm distinguishable from the other. Thus, we investigate whether real world parameters of Fano resonance coupling and enhancement with the FOLM could achieve a QBIC state.

4.2 Efficient Lattice Mode Coupling

The split modes excited in a typical asymmetric split ring resonator consist of a low frequency Fano resonance and a higher frequency dipole resonance.^[4, 13-17] The Fano resonance being the lower frequency split mode implies that coupling to the lattice mode would require a sparse array (large period), which may be inefficient. Therefore, the coupling of the ASRR was changed from capacitive coupling to inductive coupling by flipping the arms of the ASRR, as shown in the insets of Figure 4.1. The nature of coupling between the resonator arms determines the resonance frequency of the Fano resonance, which can be lower [Figure 4.1(a)] or higher [Figure 4.1(b)] than the frequency of the dipole resonance. Fano resonances in such metamaterials are characterized by anti-parallel surface currents as shown in insets of Figure 4.1(a) for a square ASRR and Figure 4.1(b) for the flipped ASRR. This brings the Fano

resonance closer to the first order lattice mode frequency (cyan dotted line), which allows for efficient resonance coupling.

Figure 4.1: Fano resonances of different aluminium resonator configurations. (a) Square configuration of end-coupled resonator arms and (b) side-coupled configuration with the resonating arms flipped. Simulations of the Fano resonance excitation allowed by asymmetry resulting from displacement of the gap by a distance $d = 3 \mu\text{m}$ from the central (symmetric) position while maintaining overall dimensions of $40 \mu\text{m} \times 40 \mu\text{m}$, an arm width of $6 \mu\text{m}$, a gap of $g = 3 \mu\text{m}$ and a period of $70 \mu\text{m}$. The insets show the simulated surface currents at the transmission minimum of the Fano resonances at (a) 0.768 THz and (b) 1.01 THz. A cyan dotted line marks the first order lattice mode $f_{LM(0,1)}$.

4.3 Electric Coupled Fano to Magnetic Coupled Fano

The ASRR shown in the inset of Figure 4.2(a) has a size of $40 \times 40 \mu\text{m}^2$, an arm width of $6 \mu\text{m}$ and a gap of $3 \mu\text{m}$. The gap is displaced by $d = 3 \mu\text{m}$ from the central vertical axis of the resonator to break the symmetry of the system and the incident radiation is polarized with the electric field parallel to the vertical axis (y-polarized). To emphasize its physical significance, we refer to the gap as the coupling distance g between the split arms. To show the change from capacitive to inductive coupling, the coupling distance is varied as shown in Figure 4.2(b). The figure shows a blue shift of a transparency peak for decreasing coupling distances, $g = 9, 5, 3 \mu\text{m}$, where the asymmetry used is $d = 1 \mu\text{m}$ for a lower transparency peak strength, as this makes the tuning of the transparency peak more visible. The blue shift of the transparency peak changes the Fano resonance from being the lower frequency split mode to the higher frequency split mode, where $g = 5$ is the threshold position when the transparency peak is exactly at the centre of the broad resonance dip. The switch from capacitive to inductive coupling can be seen in either the electric dipole (p) or the magnetic dipole (μ) moments of each arm of the ASRR obtained from simulated surface currents at the resonance frequencies of the transmission spectrum. Only transverse coupling is relevant for y-polarized ASRR illumination, which is considered here. Transverse coupling of an antisymmetric mode results in an attractive force that decreases the restoring force, and controls the resonant charge oscillation, leading to a lower resonance frequency. In contrast, transverse coupling of a symmetric mode results in repulsion that increases the restoring force, leading to a higher resonance frequency.^[9] At $g = 9 \mu\text{m}$, the dominant coupling is electric as the lower frequency split mode (Fano resonance) corresponds to the transverse coupling of electric dipoles aligned anti-symmetrically, whereas the higher frequency mode corresponds to the

symmetric transverse coupling of electric dipole moments, as shown in Figure 4.2(b-i) and (b-ii), respectively. This transmission spectrum is similar to that of a typical ASRR (without flipped resonator arms) as shown in Figure 4.1(a), where the Fano resonance is also the lower frequency split mode. At a coupling distance of $g = 3$, the dominant transverse coupling is magnetic, where the Fano resonance is now the higher frequency split mode which corresponds to magnetic dipoles aligned symmetrically, while the lower frequency split mode corresponds to antisymmetric coupling of magnetic dipoles. Though the coupling is revealed by the relative orientations of the resonant electric or magnetic dipole moments and the spectral position of the corresponding transmission resonances, the Fano resonance is still represented by antisymmetric surface currents [Figure 4.2(b-i) and (b-vi)], which trap energy in the resonators as emission from both resonator arms is prevented by destructive interference in the far field.

Figure 4.2: Fano-metamaterial. (a) Optical microscope image of the metamaterial array with schematic illustration of the incident THz field. The inset shows a unit cell containing an asymmetric split ring resonator. (b) Simulated transmission amplitude of aluminium asymmetric split ring resonators with $P = 70\ \mu\text{m}$ period, $d = 1\ \mu\text{m}$ asymmetry and coupling distances of $g = 9, 5$ and $3\ \mu\text{m}$. Their resonances are labelled (i)-(vi) and the corresponding surface currents, electric dipole moments (p) and magnetic dipole moments (μ) are shown.

4.4 Lattice Mode Coupling to Fano and Dipole Resonance

We studied the interaction between the FOLM and the metamaterial resonances of the ASRR both numerically and experimentally. Numerical investigations were conducted using a commercially available frequency-domain solver based on the finite-difference time-domain (FDTD) method, *Computer Simulation Technology (CST) Microwave Studio*. The refractive index of the silicon substrate and the conductivity of aluminium were modelled as $n = 3.42$ and $\sigma = 3.56 \times 10^7 \text{ S/m}$, respectively. The simulated and measured transmission spectra of the ASRR arrays of varying period (P) are shown in Figure 4.3. The spectra show the dipole and Fano resonances around 0.8 THz and 1.0 THz, respectively. For a lattice period of $P = 75 \text{ }\mu\text{m}$, the FOLM that is indicated by the cyan dotted line/arrow occurs at a frequency of 1.16 THz, which is higher than the Fano resonance frequency. Increasing the lattice period decreases the lattice mode resonance frequency and allows it to couple to the metamaterial resonances. Resonant coupling between the lattice mode and the Fano resonance is observed as the lattice period is increased from $75 \text{ }\mu\text{m}$ to $90 \text{ }\mu\text{m}$ [Figure 4.3(a-d)]. We see a narrowing of the Fano resonance as the lattice mode (cyan dotted line) approaches the Fano resonance with increasing lattice period. When the lattice mode frequency matches the Fano resonance at $P = 90 \text{ }\mu\text{m}$ [Figure 4.3(d)], the Fano resonance is of the narrowest linewidth. Increasing the lattice period further ($P > 90 \text{ }\mu\text{m}$) decreases the lattice mode frequency, causing a frequency mismatch between the FOLM and the Fano resonance. This decreases the strength of the Fano resonance and broadens its linewidth. Similar behaviour is observed for the dipole resonance when the lattice period is increased such that the lattice mode frequency approaches and couples to the dipole resonance frequency for periods from $P = 110 \text{ }\mu\text{m}$ to $118 \text{ }\mu\text{m}$ [Figure 4.3(e-g)]. The transmission minimum of the dipole resonance is narrowest when the lattice mode frequency matches the dipole resonance at $P = 118 \text{ }\mu\text{m}$ [Figure 4.3(g)]. As the lattice period is increased

further to $P > 118 \text{ } \mu\text{m}$, there is a frequency mismatch between the lattice mode and the dipole resonance and hence the resonances gradually decouple, thereby weakening the resonance strength, as seen in Figure 4.3(h) at $P = 122 \text{ } \mu\text{m}$. We note that the (1,1) lattice mode couples to the Fano resonance as the lattice period approaches $P = 122 \text{ } \mu\text{m}$ and a linewidth narrowing can also be seen in this case. Simulations and experiments are in good qualitative agreement. Quantitative differences regarding linewidth and strength of resonances are mainly due to limited resolution of the experimental setup ($\sim 30 \text{ GHz}$), which is unable to resolve ultra-narrow resonances.

Figure 4.3: Coupling resonances of aluminium split rings and lattice. Simulated and measured transmission amplitude of metamaterials with asymmetry $d = 3 \mu\text{m}$, coupling distance $g = 3 \mu\text{m}$ and lattice periods from $P = 75$ to $122 \mu\text{m}$. (a – d) Narrowing of the Fano resonance and (e – h) narrowing of the dipole resonance due to interaction with a lattice mode. Cyan dotted lines/arrows indicate the first order lattice mode (0,1), while green arrows indicate the (1,1) order lattice mode. Critical periods are $90 \mu\text{m}$ and $118 \mu\text{m}$, where the (0,1) lattice mode frequency matches the metamaterial’s Fano and dipole resonances, respectively.

4.5 Lattice Enhanced Q Factor and Figure of Merit

Narrow resonance features are quantitatively described by the Q factor, estimated by $Q = \omega_0/\Delta\omega$, where $\Delta\omega$ is the full width at half maximum (FWHM) of the resonance intensity and ω_0 is the resonance frequency. These resonance parameters are obtained from the transmittance spectrum, $T(\omega) = |t(\omega)|^2$, using the following equation that describes the Fano resonance^[18, 19],

$$T(\omega) = T_0 + H \frac{(W + q)^2}{(1 + q^2)(1 + W^2)}, W = \frac{\omega - \omega_0}{\Delta\omega/2} \quad (21)$$

where T_0 and H are constants, q is the asymmetry parameter which determines the resonance profile while W is a normalized expression containing the resonance frequency ω_0 and the FWHM $\Delta\omega$. The Q factor also directly relates to the losses in the metamaterial system, which can be radiative or non-radiative. But as discussed above, the losses are mainly radiative as Drude metals have high conductivity at terahertz frequencies. A common characteristic in metamaterial Fano resonances is that high- Q Fano resonances have a low intensity (transmission change) and higher intensity resonances have a lower Q . A high intensity Fano resonance at low asymmetric displacement ($d = 3 \mu\text{m}$) was used to show the effect of lattice mode coupling. We note that a higher Q factor of the Fano resonance could be achieved by optimizing the ASRR asymmetry, however, such “optimization” would disregard the practical importance of resonances that are not only narrow but that also exhibit a large resonance amplitude. In order to simultaneously optimize both resonance width and resonance depth, we consider a Figure of Merit (FoM) defined as $FoM = Q \times I$, where Q is the resonance Q factor and I is the resonant transmission change in terms of intensity. Figure 4.4(a,b) shows the Q factor and FoM as the period of the metamaterial unit cell increases, tuning the lattice mode frequency relative to the metamaterial resonances. From $P = 70 \mu\text{m}$ to $90 \mu\text{m}$, the Fano

resonance Q factor increases gradually and upon reaching the critical period for Fano coupling $P_c^{\text{Fano}} = 90 \text{ } \mu\text{m}$, it reaches a maximum of 59. A minor increase of Q factor is seen for the dipole resonance at $P = 70 \text{ } \mu\text{m}$ to $90 \text{ } \mu\text{m}$, but it increases significantly at $P > 90 \text{ } \mu\text{m}$, to a maximum of 19 at $P = 114 \text{ } \mu\text{m}$. Interestingly, the lattice mode resonantly couples to the dipole resonance at $P_c^{\text{dipole}} = 118 \text{ } \mu\text{m}$ but its maximum Q factor was obtained at $P = 114 \text{ } \mu\text{m}$. This is because the resonance interaction occurs near the half maximum of the high-intensity dipole resonance for $P = 114 \text{ } \mu\text{m}$ and at its transmission minimum for $P = 118 \text{ } \mu\text{m}$, resulting in squeezing of FWHM and tip of the dipole resonance, respectively. Therefore, the Q factor at $P = 114 \text{ } \mu\text{m}$ is slightly higher than at the critical period, $P_c^{\text{dipole}} = 118 \text{ } \mu\text{m}$. A similar trend is seen for the FoM , which also increases with increasing lattice period as the lattice mode frequency approaches the metamaterial resonances, reaching a maximum value of $FoM = 33$ for the Fano resonance at $P_c^{\text{Fano}} = 90 \text{ } \mu\text{m}$ and a maximum of $FoM = 15$ for the dipole resonance at $P = 114 \text{ } \mu\text{m}$. Figure 4.4(c) shows the simulated transmission amplitude spectra as a function of the lattice period. It clearly depicts the resonance narrowing as the lattice mode approaches and then matches the ASRR Fano and dipole resonance frequencies at the critical periods of 90 and 118 μm .

Figure 4.4: Lattice-dependence of resonant metamaterial properties extracted from simulations. (a) Q factor and (b) figure of merit ($FoM = Q \times I$, with resonant transmission intensity change I) of the dipole (black) and Fano (red) resonances at different lattice periods of the aluminium metamaterial with asymmetry $d = 3 \mu\text{m}$ and coupling distance $g = 3 \mu\text{m}$. (c) Transmission amplitude as a function of the metamaterial's period and frequency of the incident THz wave. The metamaterial resonances are narrowest when they coincide approximately with the lattice mode $f_{\text{LM}(0,1)}$ for critical periods $P_c^{\text{Fano}} = 90 \mu\text{m}$ and $P_c^{\text{dipole}} = 118 \mu\text{m}$ (dashed lines).

4.6 Symmetry Broken Bound States in the Continuum

To determine the nature of the Fano resonance and the ability of its enhancement due to FOLM coupling to achieve a QBIC state under realistic parameters, an illumination-angle-dependent simulation is performed assuming ideal metallic resonators made from perfect electric conductor (PEC). Figure 4.5(a) shows the transmission amplitude as a function of

illumination angle and frequency for arrays of symmetric ($d = 0$) PEC metamaterial resonators with coupling distances of $g = 3, 5$ and $9 \mu\text{m}$ and otherwise of the same geometry as in Figure 4.2. Similar to Figure 4.2(b), the coupling distance determines the coupling nature (magnetic or electric) of the metamaterial and hence the spectral positions of the dipole resonance, the BIC/QBIC/Fano resonance and the transmission peak in between. As the angle of incidence increases, we can see the collapse of the symmetry protected BIC at normal incidence to a resonance with a finite linewidth, at $0.97, 0.93$ and 0.90 THz for $g = 3, 5$ and $9 \mu\text{m}$ respectively [red arrows in Figure 4.5(a)]. The QBIC state is where the BIC just collapses and loses its zero linewidth and infinite lifetime. This happens at a slight perturbation of the symmetry protected system as illustrated by Figure 4.5(b), where we see the QBIC with an ultra-narrow linewidth for 2° oblique illumination of the symmetric PEC structure (black lines). To facilitate measurements at normal incidence, another method to induce a QBIC resonance is to break the structural symmetry of the resonator. This is illustrated by Figure 4.5(b) for normal illumination of PEC ASRR arrays, where the gaps are displaced from the resonator's central vertical axis by the asymmetry parameter $d = 0.25 \mu\text{m}$ (red dashed lines). Both BIC perturbations, either a small illumination angle or a small structural asymmetry, yield QBIC at almost identical spectral positions [Figure 4.5(b)] and similar behaviour has also been reported by other groups.^[20-22] Figure 4.5 also illustrates that the QBIC can be tuned across the broad continuum by changing the coupling distance between the components of the metamaterial unit cell, from high frequencies to an EIT-like spectrum and low frequencies.

Figure 4.5: Excitation of bound metamaterial states in the continuum by symmetry breaking. Simulations are shown for metamaterial arrays with period $P = 70 \mu\text{m}$ consisting of PEC resonators with different coupling distances of $g = 3, 5$ and $9 \mu\text{m}$. (a) Transmission amplitude spectra of symmetrically coupled resonators ($d = 0 \mu\text{m}$) as a function of angle of incidence in the xz -plane. Symmetry protected BIC are shown by red arrows at normal incidence. (b) Transmission amplitude spectra of QBIC excited by illumination of the symmetric structures with 2° angle of incidence (solid lines) or at normal incidence by introduction of a small structural asymmetry $d = 0.25 \mu\text{m}$ (dashed lines). An example of the ultra-narrow resonance of the QBIC is shown and magnified in the inset of $g = 3 \mu\text{m}$.

4.7 Diverging Nature of Quasi-Bound States in the Continuum Q Factor

As the perturbation is reduced towards zero to approach the symmetry-protected BIC, the line width becomes zero and the Q factor diverges to infinity, as shown in Figure 4.6. Our simulations show that both oblique illumination of symmetric resonators [Figure 4.6(a)] and structural asymmetry of resonators at normal incidence [Figure 4.6(b)] can control the Q factor of QBIC/Fano resonances in PEC metamaterials by at least two orders of magnitude. While the Q factor could in principle diverge to infinity under ideal conditions, under real world conditions, losses and detector resolution limit the achievable and detectable Q factors. This effect of losses is shown for aluminium resonator arrays with a coupling distance $g = 3 \mu\text{m}$, which achieved maximum Q factors that are about two orders of magnitude lower than those calculated for PEC resonator arrays. For these aluminium resonator arrays, the highest Q factor resonances, that occur at near-normal incidence [Figure 4.6(a)] / low asymmetry [Figure 4.6(b)], suffer from low resonance intensity. Figure 4.6(c) shows a comparison of Q factors between arrays of PEC and aluminium ASRRs with asymmetry $d = 3 \mu\text{m}$ and coupling distance $g = 3 \mu\text{m}$ for different lattice periods, where FOLM coupling and enhancement of the Fano/QBIC resonance occurs at $P = 89$ and $90 \mu\text{m}$ for PEC and aluminium ASRRs, respectively. While FOLM coupling enhances the Q factor, the maximum Q factor calculated with FOLM coupling under real world conditions is still about two orders of magnitude lower than that of the QBIC under ideal low-asymmetry PEC conditions. For aluminium resonators, our results indicate that the three different optimization strategies – small angle of incidence onto symmetric resonators, normal incidence onto low-asymmetry resonators and FOLM coupling – yield comparable maximum Q factors, which are limited by non-radiative losses in aluminium. We note that the resonators used for FOLM coupling have a significant asymmetry of $d = 3 \mu\text{m}$ – and thus high

resonance intensity – for experimental detection and suffer from ohmic losses in the metal as well as a small amount of substrate absorption. Very low asymmetry resonators made from low-loss materials will require high fabrication accuracy to avoid inhomogeneous broadening and precise matching of the FOLM to the ultra-narrow Fano/QBIC resonance to achieve resonance enhancement.

Figure 4.6: Q factor of the simulated Fano resonance as a function of (a) angle of incidence θ , (b) asymmetry d and (c) period P . (a, b) The Q factor of PEC resonator arrays diverges to infinity when incidence angle and asymmetry both approach 0 as the resonance is protected by symmetry in this case. Results for aluminium resonator arrays with a coupling distance of $g = 3 \mu\text{m}$ are shown for comparison. (c) Comparison between ideal PEC and realistic aluminium resonator arrays with asymmetry $d = 3 \mu\text{m}$ and coupling distance $g = 3 \mu\text{m}$ for different periods, where FOLM coupling is indicated by a dashed line.

4.8 Lattice Mode Enhanced Electric and Magnetic Fields

To further investigate the Q factor enhancement of the metamaterial resonances due to FOLM coupling, we performed numerical simulations of the electric and magnetic field under lattice matched and mismatched conditions of both the Fano and dipole resonances. Figure

4.7(a-d) shows the electromagnetic field distributions of the Fano resonance mismatched and matched to the first order lattice mode at $P = 70$ and $90 \mu\text{m}$, respectively. Under lattice matched conditions we observe some electric field enhancement on the ends of the left resonator arm and along the gap. Since the Fano resonance arises from the inductively coupled resonator arms, we also see a strong enhancement of the magnetic fields in the gap. This enhancement due to coupling to the lattice mode strengthens the confined light in the gap and the FOLM-enhanced fields are evidence of reduced radiative losses, leading to the high Q lattice matched metamaterial resonance. Figure 4.7(e-h) shows the electromagnetic field distribution of the dipole resonance mismatched and matched to the first order lattice mode at $P = 70 \mu\text{m}$ and $P = 118 \mu\text{m}$. Similar results can be seen in the fields of the dipole resonance, where lattice matching yields stronger overall excitation of the structure. While only the longer resonator arm is strongly excited without lattice matching, FOLM-coupling of the dipole resonance at $P = 118 \mu\text{m}$ results in substantial excitation of both resonator arms. Magnetic field enhancement due to lattice-matching is seen along the inner edge of each C-shaped resonator arm, which is evidence of increased currents in each resonator arm. However, the magnetic field within the gap between the resonator arms remains weak, and indeed the magnetic fields generated by a pair of identical electric dipoles is expected to cancel here.

Figure 4.7: Lattice-induced field-enhancement. The near field total electric and magnetic field amplitude, $|E|$ and $|B|$, of the Fano and dipole resonance under lattice mismatched ($P = 70 \mu\text{m}$) and lattice matched conditions (Fano: $P = 90 \mu\text{m}$; dipole: $P = 118 \mu\text{m}$) for aluminum split ring arrays with asymmetry $d = 3 \mu\text{m}$ and coupling distance $g = 3 \mu\text{m}$. All maps of the same field share a color scale with the same range. Field enhancement is marked by white dashed ovals under lattice matched conditions.

4.9 Conclusion

In summary, lattice mode matching was performed on a terahertz asymmetric resonator with a Fano resonance as the higher frequency split mode. This was done by transverse coupling of symmetric magnetic dipole moments. The lattice mode traps electromagnetic fields in the plane of the metamaterial array and interferes with the metamaterial response, strengthening the resonant field confinement and reducing radiative loss. This lowered radiative loss yields a higher Q factor resonance. Here, lattice mode coupling increases the Q factor and Figure of Merit of the Fano transmission resonance by several times. We have shown that the Fano resonance originates from a symmetry protected BIC and radiates as a quasi-BIC state. We have shown that such quasi-BIC/Fano resonances can be tuned across the broad

dipolar continuum by changing the coupling distance of the resonators. Coupling to the first order lattice mode provides a simple and general method for increasing the Q factor of metamaterial resonances for applications such as sensing, narrow band filtering and lasing spasers. The narrow gaps in this high frequency Fano design could also be used as micro channels for microfluidic sensing type applications.

4.10 Reference

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CHAPTER 5

Nano-dielectric-induced active quasi-bound states in the continuum: A flexible metasurface platform for terahertz switching and sensing applications

5.1 Introduction

In this chapter, we use strips of photoactive semiconducting material to introduce an asymmetry in a metamaterial based on symmetric metallic resonators, namely split-ring resonators (SRRs).^[1] The incorporation of the semiconducting material does not only result in a QBIC resonance but also allows selective modulation of the resonance. The combination of an active superstrate layer on a metallic resonator enables the resonant unit cell to remain small compared to the wavelength, which is not possible in an all-dielectric configuration. This approach could potentially be used with any active dielectric material on any planar symmetric resonator that supports a BIC mode. Here, we chose Ge to demonstrate ultrafast switching and modulation of the QBIC resonances. The Ge strips resembles microchannels, where an analyte could flow for sensing. We provide an optimization model for this system which can be used to design metasurfaces with a desired combinations of Q factor and Figure of Merit (FoM).

5.2 BIC in Split Ring Resonator

Throughout this work, we will consider the properties of metamaterials illuminated at normal incidence (unless stated otherwise) by vertically (y) polarized THz waves. Before considering QBICs in metamaterials with asymmetry imposed by dielectric strips on symmetric metallic SRRs, we will consider the BIC of the symmetric structure without the dielectric strip. This investigation characterizes the BIC before any symmetry breaking

perturbations. The dimensions and geometry of the symmetric SRR unit cell are shown in Figure 5.1(a-i). It has a 95 μm period, 80 μm edge length, 6 μm resonator line width and 4 μm split gap. Assuming the absence of absorption losses, an eigenmode analysis was carried out using COMSOL Multiphysics reveals two eigenmodes (white dashed lines) as shown in Figure 1(a-ii), which are also seen in the incidence-angle-dependent simulations of the structure's transmission spectrum by CST Microwave Studio (CST) shown on the same figure. The lossless parameters are as follows: perfect electric conductor (PEC) is chosen for the 200-nm-thick SRR metalized layer and a substrate of 50- μm -thick cyclic olefin copolymer (COC) with a refractive index of $n_{\text{COC}} = 1.52$.^[2, 3] With these parameters, we obtained a dipole mode at 0.91 THz and a narrow mode at 0.754 THz in the transmission spectrum 2D map. The resonance frequency and the eigenfrequency of the narrow mode found using CST and COMSOL simulations match quite well, with a narrow high- Q mode at about 0.754 and 0.747 THz, respectively. The simulations are done between high symmetry points of the Brillouin zone from Γ towards X. It can be seen from the transmission amplitude of the incidence-angle-dependant simulations that the narrow resonance mode vanishes at normal incidence (Γ point, where $k_x = 0$). This together with the diverging Q factor at the Γ point seen in Figure 5.1(a-iii) are characteristics of a symmetry protected BIC, which decouples from free space and cannot be observed experimentally with an entirely symmetric configuration. The Q factor extracted from the eigenmode calculation follows an inverse square trend ($Q \sim k_x^{-2}$) as it moves further away from the Γ point, which is also reported in other BICs.^[4] Another feature of a BIC is its vortex centre in the polarization of the far-field radiation, characterized by a topological charge.^[5, 6] The topological charge (q), which describes the number of winds around the BIC at the Γ point in $\mathbf{k}$ space, is defined as:

$$q = \frac{1}{2\pi} \oint_C d\mathbf{k} \cdot \nabla_{\mathbf{k}} \phi(\mathbf{k}), \quad (22)$$

where $\phi(\mathbf{k}) = \arg [E_x(\mathbf{k}) + iE_y(\mathbf{k})]$ is the angle of the polarization vector and C is a closed path in $\mathbf{k}$ space that goes around the BIC in the counterclockwise direction. The electric fields $E_x(\mathbf{k})$ and $E_y(\mathbf{k})$ form the polarization ellipse and are obtained from COMSOL to plot the evolution of the polarization angle $\phi(\mathbf{k})$ in Figure 5.1(a-iv) and to calculate q . The black circular lines in the same figure show the polarization direction, *i.e.* the direction of the major axis of the polarization ellipses. The polarization vector winds around the Γ point and the polarization angle changes by $+2\pi$ on a counterclockwise closed path around the Γ point, which corresponds to a positive topological charge, $q = +1$.

Any symmetry-breaking perturbation of the BIC allows access to a narrow high- Q mode. This strategy is commonly followed by creating an asymmetry between the two constituent resonating arms by shifting one or both of the gaps.^[7] In contrast, the method demonstrated here maintains the symmetry of the resonator and incorporates a thin semiconducting layer on a portion of the unit cell. The chosen semiconducting material is germanium (Ge) with a refractive index of $n_{\text{Ge}} = 4$. To disrupt the symmetry, a 500-nm-thick Ge strip of width $s = s_L + s_R$ is used to cover (i) part of the left (L) half of the unit cell or (ii) all of the left half and part of the right (R) half of the unit cell, as shown in Figure 5.1(b). Starting from the centre of the unit cell, as the Ge strip is extended to cover the unit cell's left half, the unit cell becomes increasingly asymmetric and the QBIC emerges and redshifts in the transmission spectrum, from the BIC frequency at 0.754 THz to 0.66 THz when the left half of the unit cell is fully covered. Further widening the strip into the right half results in a significant redshift as Ge coverage of the resonator's capacitive gap causes a capacitance increase and thus a resonance frequency decrease ($\omega_0 \approx 1/\sqrt{LC}$). The resonance frequency continues to redshift until the

unit cell is completely covered with Ge, which restores the symmetry of the structure, causing the QBIC to recover to a BIC at 0.61 THz. Thus, a complete absence of the strip and complete strip coverage (and indeed any symmetric coverage, $s_L = s_R$) yield a BIC. Interestingly, the QBIC resonance narrows and vanishes as these cases are approached.

Figure 5.1: Hidden BIC resonance of an array of symmetric SRRs and a dual BIC configuration. (a)(i) Dimensions of the unit cell consisting of a PEC resonator on a cyclic olefin copolymer (COC) substrate. (ii) Transmission amplitude spectra and eigenfrequencies (white dashed lines) of the symmetric SRR array. The red arrow shows the symmetry protected BIC at normal incidence (Γ point), and the QBIC resonance observed at oblique incidence ($0 - 12^\circ$, away from the Γ point, $k_x > 0$). (iii) Calculated Q factor of the QBIC resonance diverging to infinity at its symmetry protected Γ point. (iv) The angle of the polarization vector in k space with black lines illustrating the

polarization direction at the BIC frequency. The BIC corresponds to a topological charge $q = +1$ at the Γ point. (b) Transmission amplitude spectra as a function of the width of an additional 500-nm-thick Ge strip covering part of the left (s_L) and right (s_R) halves of the unit cell. A BIC is present in symmetric cases, e.g. absence of the Ge strip and complete Ge coverage of the unit cell.

5.3 QBIC in Symmetric Split Ring Resonator

Ge has an indirect bandgap of 0.66 eV and a larger intrinsic carrier concentration and higher carrier mobility than silicon. Its ultrafast carrier dynamics and high absorption coefficient have also been appealing for photonic devices such as photodetectors or solar cells.^[8, 9] As such, Ge is a suitable photoactive material for modulating or switching metamaterial resonances, removing the need for electrical contacts. The COC substrate not only supplements the functionality by giving the device flexibility as shown in Figure 5.2(a-i) but also minimizes the loss by having excellent optical characteristics (refractive index $n = 1.52$ and loss tangent of $\tan \delta \sim 0.0006$)^[2, 3] at terahertz frequencies. Moreover, its refractive index is low enough to avoid lattice modes near the QBIC frequency^[10]. Samples were fabricated with a two-step photolithography process with a maskless aligner by our collaborators in RMIT. The first step photolithography is for the gold resonators while the second step is for the Ge strips. Images of the fabricated metamaterial array and its SRR unit cell are shown in Figure 5.2(a-ii). The unit cell dimensions match those of Figure 5.1(a), with gold being used instead of PEC for the SRRs and with a Ge strip of width $s = s_L = 47.5 \mu\text{m}$, will now be used in the subsequent investigation and demonstrations. The addition of the semiconducting strip, which removes the yz -plane mirror symmetry at the centre axis of the resonators, enables different excitation of the left and right resonator arms by normally incident y -polarized THz waves. This is illustrated by Figure 5.2(b), which shows the electric field E_z on a two-unit-cell cross-section of the metamaterial along the gap (black dotted rectangle) for the cases with and without

Ge strip at the QBIC resonance frequency (0.66 THz). The presence of the Ge strip leads to excitation of an asymmetric mode in the left (L) and right (R) resonator arms, which cannot be excited in the symmetric case. The asymmetric excitation is associated with strong local fields as (approximately) destructive interference in the far-field traps energy in the metamaterial structure. However, the mode is not perfectly anti-symmetric, slightly stronger fields can be seen in the Ge-covered half of the unit cell. It is this deviation from the perfectly anti-symmetric BIC mode that allows the asymmetric QBIC mode to leak and couple to the continuum as a far-field radiation. This slight asymmetry of the excitation can also be interpreted as a resonance frequency mismatch of the two resonating arms and an interference, where the resonance frequency ω_0 of the Ge-covered resonator arm is lowered. Both modes are plotted on the same scale, and thus a comparison of the field maps shows that the symmetric local fields excited in the symmetric structure without the Ge strips are substantially weaker. The symmetric mode does not change much throughout the whole feature of the broad resonance, and constructive interference in the far-field implies that it is strongly coupled to the far-field and cannot trap much energy in the metamaterial device.

Figure 5.2: Flexible QBIC metaphotonic and simulated electric fields accompanied by its transmission. (a) (i) Flexible QBIC metaphotonic filter and sensor. (ii) Optical microscope image of the metaphotonic device with Ge strips of width $s = s_L = 47.5 \mu\text{m}$ and thickness $h = 500 \text{ nm}$ covering half of each unit cell as shown by the inset. (b) Simulated transmission amplitude spectra and field maps for devices with and without Ge strips. The field maps show the z -polarized electric field in the cross-sectional plane marked on the inset of (a-ii) across two-unit cells when the structure is illuminated by normally incident y -polarized electromagnetic waves at 0.66 THz . The black dotted rectangles represent the SRR gap, and L (R) represents the left (right) half of the unit cell.

5.4 Ultrafast QBIC Filter

The narrow QBIC resonance of the metal-semiconductor metamaterial structure could be exploited for spectral filtering, while the thin semiconductor layer offers an opportunity for active control of the device. Active control of the QBIC resonance is first investigated by CST simulations by changing the conductivity of Ge and then experimentally by optically pumping the device to excite charge carriers in the Ge strip. The increase of Ge conductivity due to photoexcitation of carriers in the conduction band changes the interaction between the incident THz waves and the metaphotonic device. As the Ge strip becomes more metallic, the interaction between the THz waves and the resonator, which is buried under Ge, is suppressed. Hence, the metamaterial changes from an SRR array to a strip grating coupled to half SRRs. The conductivity of Ge is varied from $\sigma = 1$ to 4×10^7 S/m, which is about the conductivity of gold. Simulations of the transmission amplitude as a function of frequency and conductivity presented in Figure 5.3 reveal three regimes of operation of the metaphotonic device: (a) QBIC bandstop, (b) intermediate switch off and (c) extraordinary transmission (ET) bandpass. Figure 5.3(a) shows a narrow bandstop modulation at 0.66 THz as the conductivity increases from 0 to 10^3 S/m, at the QBIC resonance that arises from the symmetry breaking of the BIC phenomenon. Figure 5.3(b) shows a transitional resonance switch off between the two operations, bandstop and bandpass, as the conductivity ranges from 6×10^3 to 2×10^5 S/m. Figure 5.3(c) shows how the transmission spectrum develops a bandpass as the conductivity of the Ge strips is increased further. This conductivity increase causes the Ge strips to act as a grating that couples to the remaining arm of the SRR. This coupling results in metamaterial-induced extraordinary transmission at 0.7 THz, which is below the range of the conventional ET. Conventional ET follows the equation^[11-13], $f_{ET} = c/n_{sub}P = 2.08$ THz, where c is the

speed of light, n_{sub} is the refractive index of the substrate and P is the period (lattice constant) of the metamaterial. These simulations show that our metaphotonic device has the potential to switch between a bandstop and a bandpass filter, which a slight resonance shift from 0.66 THz to about 0.7 THz. However, this requires an active material with high photoconductivity.

Figure 5.3: Tunable terahertz metaphotonic filter. Simulated transmission amplitude as a function of frequency and Ge conductivity σ for the device of Fig. 2a. (a) Narrow bandstop filter modulation of the QBIC resonance from $\sigma = 0$ to 10^3 S/m. (b) Intermediate transition ‘off’ state of the bandstop and bandpass operation at $\sigma = 6 \times 10^3$ to 2×10^5 S/m. (c) Narrow bandpass filter modulation of the metamaterial induced extraordinary transmission from $\sigma = 4 \times 10^5$ to 4×10^7 S/m

The filtering and switching characteristics of the metaphotonic device have been measured by terahertz time-domain spectroscopy (THz-TDS) using an optical pump and a terahertz probe (OTTP) as described in the experimental section. The device is illuminated with a pulsed optical pump beam of 800 nm wavelength at different average power levels of 200, 600 and 1200 mW (pump fluences of 254.6, 763.9 and 1273.2 $\mu\text{J}/\text{cm}^2$, respectively). As shown by Figure 5.4(a), optical pumping yields substantial changes in the structure’s transmission amplitude spectrum at the QBIC resonance (shaded region). The QBIC resonance becomes

weaker with increasing pump fluence as predicted by the simulations shown in Figure 5.3(a), i.e. the optical pump switches the narrow stopband of the filter off. We note that we limited the maximum experimental pump fluence to $1273 \mu\text{J}/\text{cm}^2$ to avoid optical damage to the sample. Within the safe range of fluences, the increase in Ge conductivity is sufficient to suppress the QBIC resonance substantially, but the resonance does not vanish completely. While we are unable to experimentally demonstrate the simulated bandpass filter operation of Figure 5.3(c) with this Ge-based device, the bandpass regime may be accessible with other materials such as semimetals.^[14, 15] The spectra of Figure 5.4(a) were recorded with an optical pump delay of 0 ps. Within experimental accuracy, Figure 5.4(c-i), which shows the transmission amplitude modulation as a function of pump-probe delay, reveals that the maximum transmission modulation and Ge conductivity occur at this 0 ps delay, i.e. when the optical pump pulse interacts with the centre surface of the photoactive sample while the THz probe pulse passes through the sample.

The change in transmission amplitude between the presence (t_{pump}) and the absence (t_0) of an optical pump is shown in Figure 5.4(b). The maximum absolute transmission amplitude change obtained at the QBIC resonance is $t_{\text{pump}} - t_0 = 0.16$, corresponding to modulation of $\frac{t_{\text{pump}} - t_0}{t_0} \times 100\% = 75\%$. At higher pump fluence, we also observed a large transmission change at higher frequencies, which is due to the broadening of the dipole mode and does not significantly affect the resonance amplitude and the switching capabilities of the device. The observed pump-induced modulation of the transmission amplitude is significant at the QBIC resonance frequency and small at the dipole resonance frequency, as highlighted by the red dashed lines in Figure 5.4(b). Thus, we observe optical switching of a single resonance in the QBIC device.

The evolution of the transmission amplitude as a function of pump-probe delay carries information about the photoconductive carrier response in the metaphotonic device, i.e. the excitation and relaxation dynamics of the photo-carriers in the Ge strip, see Figure 5.4(c-i). The pump pulse photoexcites carriers to the conduction band, resulting in a photoexcitation maximum at a delay of about 0 ps. The photoexcitation and relaxation are dependent on pump fluence, as the photoexcitation peak of $\Delta t/t_0$ increases with increasing pump fluence, where $\Delta t = t_{pump} - t_0$ in the time domain. However, it should saturate exponentially at high pump fluence as the number of carriers that can be photoexcited to the conduction band is finite. An upper limit for the relaxation time can be extracted through a single exponential fit and the time constant τ_1 is presented in Table 1 for different pump fluences.^[16-18] We note that, due to oblique pump illumination, the pump pulse takes around 4-5 ps to cross the probed sample region, which is comparable to the full-width half maximum (FWHM) of the observed modulation. Thus, the response of the metaphotonic device is at least as fast as indicated by the fitted time constant but could also be much faster than that.

Table 1. Exponential time constants extracted from fitting Figure 5.4(c-i) at different pump fluences.

Pump fluence [$\mu\text{J}/\text{cm}^2$]	254.6	763.9	1273.2
τ_1 [ps]	2.04 ± 0.14	1.96 ± 0.05	1.92 ± 0.03

Figure 5.4(c-ii) shows the temporal evolution of the QBIC resonance at different timestamps for a fixed pump fluence of $763.9 \mu\text{J}/\text{cm}^2$. At peak photoexcitation, the conductivity and the resulting transmission modulation at the QBIC resonance are the largest. As the carriers recombine, the Ge conductivity reduces and the QBIC resonance recovers, as shown in Figure

5.4(c-ii) from 0 to 7 ps. This demonstrates ultrafast switching of the QBIC resonance, which recovers within 7 ps while the dipole resonance remains almost unchanged. Our results also demonstrate how either pump-probe delay or pump fluence can be used to modulate a QBIC resonance.

Figure 5.4: Optical control of the bandstop filter function of the device of Fig. 2a. (a) Measured THz transmission amplitude spectra at different optical pump fluences. (b) Absolute change of the transmission amplitude induced by the optical pump. The grey shaded area and red dashed line highlight the QBIC resonance while the red dashed arrow points to negligible absolute modulation at the dipole resonance. (c) Measured optical pump-induced modulation. (i) Normalized transmission amplitude change due to optical pump at the peak of the time-domain THz signal for different pump fluences. (ii) Transmission amplitude spectra measured at various time delays between the optical pump and THz probe at 764 $\mu\text{J}/\text{cm}^2$ pump fluence, showing temporal modulation with complete recovery of the QBIC resonance within 7 ps.

5.5 Microchannel QBIC Refractive Index Sensor

Recently, I. Al-Naib^[1] reported refractive index sensing based on breaking the symmetry of an SRR through an analyte layer. Inspired by his work, our BIC-based refractive index sensor design uses a Ge layer on half of the unit cell to form a microchannel for an analyte to flow over the uncovered half, as shown in the inset of Figure 5.5. In such devices, the optical path length difference for wave propagation through the analyte and the material covering the other half of the unit cell causes the symmetry breaking of the BIC and the spectral shift of the resulting QBIC. The larger the refractive index difference (Δn) and the layer thickness (h), the greater the optical path length difference $\Delta n \cdot h$ and the associated symmetry breaking and resonance QBIC shift away from the BIC's Γ point. Having the semiconducting strip already in place improves and ease up the fabrication for device integration. The choice of the semiconducting material enables device optimization for operation in a desired refractive index range, where the QBIC is narrow. Figure 5.5(a) illustrates the working principle of the device by showing how the transmission amplitude spectrum depends on the analyte's refractive index. The thickness of the superstrate (Ge and analyte) is kept constant at $h = 500$ nm. Since the refractive index of Ge is 4, we observe a collapse of the QBIC's linewidth for increasing and decreasing values of n as it approaches the BIC at $n = 4$. The horizontal white dashed line marks the eigenfrequency of the BIC (0.607 THz) calculated in COMSOL when the metamaterial is symmetric and completely covered with Ge, which matches well with the vanishing of the resonance in the transmission amplitude simulation in CST. Figure 5.5(b) shows the resonance shift as a function of the analyte's refractive index, and we can extract the sensitivity of the sensor from the gradient of the linear dispersion. In order to avoid discontinuities in the superstrate around the 200-nm-thick gold resonators, we simulate larger superstrate thicknesses of 300 to 500 nm to characterize the device's sensitivity. The sensitivity

increases with increasing superstrate thickness, but this effect will eventually saturate as reported for other metamaterial-based refractive index sensors.^[19, 20] The sensitivity obtained with a 500-nm-thick superstrate is $\Delta f/\Delta n = -24.5$ GHz/RIU. The sensitivity in terms of wavelength is $\frac{d\lambda}{dn} = -\frac{c}{f_0^2} \frac{df}{dn} = 1.7 \times 10^4$ nm/RIU, where c is the speed of light and $f_0 = 0.66$ THz is the QBIC resonance frequency. This shows the versatility of the metaphotonic device design as a refractive index sensor for analyte layers of nanoscale thickness. The freedom to choose the superstrate material that forms the microchannels allows the BIC and nearby high- Q QBIC to be shifted depending on device, integration, resolution, and application requirements.

Figure 5.5: Terahertz nanoscale refractive index sensor. (a) Simulated transmission amplitude spectra showing the collapse and revival of the BIC resonance mode with changing refractive index of an analyte placed in microchannels separated by the Ge strips. The refractive index of Ge is 4 (vertical dashed line), and the calculated BIC resonance from COMSOL is 0.607 THz (horizontal dashed line). (b) The spectral shift of the QBIC resonance as a function of the analyte's refractive index for different thicknesses of the superstrate (Ge strip and analyte) $h = 300, 400$ and 500 nm. The device sensitivity in terms of frequency shift per refractive index unit is obtained from the slope through a linear fit. The inset shows the device with analyte flowing through microchannels in between the Ge strips.

5.6 Device Design and Optimisation

A QBIC that arises from breaking the symmetry of the unit cell with a dielectric strip can be optimized by adjusting the geometrical parameters of the dielectric strip, without changing the geometry of the metallic resonator. This concept allows upgrading the functionality of any existing planar symmetric resonator design, that supports a BIC mode, with any available dielectric. This is illustrated in Figure 5.6, which shows the dependence of the QBIC resonance on the strip's (a) width, (b) thickness and (c) material permittivity/refractive index. Simulated and measured transmission amplitude spectra of the metaphotonic device with a Ge thickness of $h = 500$ nm show that the QBIC resonance red-shifts (0.7 to 0.66 THz) and increases in amplitude as the strip width s increases from 16 to 47.5 μm [Figure 5.6(a)], where the 47.5- μm -wide (half-Ge) strip covers half of the unit cell. In contrast, the amplitude of the dipole resonance remains unchanged. The half-Ge strip structure was chosen for in-depth experimental characterization as it provides a resonance with a large amplitude and suitable linewidth for our measurement setup with a spectral resolution down to 30 GHz or more. Similarly, as the thickness of the half-Ge strip is varied from 200 to 700 nm [Figure 5.6(b)], the QBIC resonance is redshifted (0.71 to 0.63 THz) and its amplitude increases while the dipole resonance's amplitude remains the same. Thinner Ge could be advantageous for photoactive control as it requires less optical pump fluence to increase its conductivity, however, thinner Ge also yields a weaker QBIC resonance. Considering this trade-off, a thickness of 500 nm was chosen. Measured and simulated resonances in Figure 5.6(a) and (b) match well in terms of spectral position. The contrast of experimental spectra is limited by the 30 GHz spectral resolution of the THz-TDS setup. Figure 5.6(c) illustrates that any dielectric can be used to obtain a QBIC resonance, for resonance optimization as well as sensing

applications (see the previous section). The larger the strip's permittivity, the thinner the strip can be for a measurable QBIC resonance, indicating that thinner strips made from a higher-permittivity semiconductor should be suitable for optical QBIC control at lower pump fluence. Other dependence such as strip translation and additional results on strip width variation are shown in Figure 5.7 and Figure 5.8, respectively.

Figure 5.6: Simulated (top) and measured (bottom) transmission amplitude for devices with (a) varying Ge strip widths from $s = 16$ to $47.5 \mu\text{m}$ for a fixed Ge thickness of $h = 500$ nm, (b) Ge strips of varying thickness from $h = 200$ to 700 nm with a fixed width of $s = 47.5 \mu\text{m}$ and (c) strips of materials with permittivity from $\epsilon = 1$ to 80 with fixed thickness $h = 500$ nm and fixed width $s = 47.5 \mu\text{m}$.

Figure 5.7: The effect of Ge strip translation on the simulated transmission amplitude spectrum. A Ge strip of width $s = 16 \mu\text{m}$ and thickness $h = 500 \text{ nm}$ is translated away from the centre of the unit cell by different distances d_x . The striped shaded area represents the symmetric strip area that cannot contribute to asymmetry. The remainder of the Ge strip area (not striped) contributes to asymmetry and its location is given by $d_{x,\text{asym}}$.

Figure 5.8: Simulated transmission spectra for SSR metamaterials with different Ge strip widths $s = 16, 30$ and 47.5 μm (half of the unit cell) at (a) 200 and (b) 700 nm strip thickness. The respective strip width s is shown in (c).

In order to quantify and compare QBIC resonance characteristics, we fitted the transmittance spectra, $T(\omega) = |t(\omega)|^2$, as a Fano resonance T_F (the QBIC resonance) on a Lorentzian background T_d (the dipole resonance).

$$T(\omega) = T_d + T_F \quad (23)$$

$$T_d = T_0 - I_d \frac{(\gamma_d/2)^2}{(\omega - \omega_{d0})^2 + (\gamma_d/2)^2} \quad (23a)$$

$$T_F = -I_F \frac{(W + q)^2}{(1 + q)^2(1 + W^2)}, \quad W = \frac{\omega - \omega_{F0}}{\gamma_F/2} \quad (23b)$$

where the subscripts d and F correspond to dipole and Fano respectively, ω_0 , γ and I are frequency, FWHM and normalized intensity of the corresponding resonance, T_0 is the baseline shift of the whole spectrum, and q is the asymmetry parameter that determines the QBIC resonance profile.

The radiative losses of the QBIC resonance can be estimated by the Q factor, $Q = \omega_{F0}/\gamma_F$. Another parameter of practical importance is the resonance intensity (depth) I , which can be extracted from the QBIC resonance peak and dip of the transmittance spectrum. As there is a trade-off between Q factor and intensity of the QBIC resonance,^[7] we consider their product as a figure of merit, $FoM = Q \times I$, in order to find the optimal trade-off. The Q factor, intensity and figure of merit of the QBIC resonance all depend on the strip-induced asymmetry.

Here we describe this asymmetry α in a generalized form as the product of contributions associated with the strip area, its optical thickness, and its interaction with the metallic resonator.

$$\alpha = \alpha_{\text{Area}} \times \alpha_{\text{Optical}} \times \alpha_{\text{SRR}} \quad (24)$$

$$\alpha_{\text{Area}} = \frac{2|A_L - A_R|}{A_{\text{unit cell}}} \quad (24a)$$

$$\alpha_{\text{Optical}} = \left| \frac{n_{\text{strip}} - n_o}{n_o} \right| \frac{h}{1 \mu m} \quad (24b)$$

$$\alpha_{\text{SRR}} = 2 - \left| \frac{4d_{x,\text{asym}}}{P_x} \right| \quad (24c)$$

Any mirror-symmetric unit cell consists of two halves, “left” and “right”, which are mirror images of each other. Asymmetry results from any area of asymmetric strip coverage of the two halves and this are quantified as α_{Area} , the fraction of the unit cell that is covered asymmetrically. For a single strip oriented parallel to the symmetry axis (y-axis), it is twice the

difference between left and right strip areas, $A_{L,R} = s_{L,R} \times P_y$, normalized by the area of the unit cell, $A_{\text{unit cell}}$. As illustrated by Figure 5.9(a), any part of a strip that is symmetric with respect to the symmetry axis does not contribute to area asymmetry (striped region) and the largest asymmetry of 1 corresponds to the case when the strip covers one half of the unit cell entirely, but not the other. This behaviour is clearly seen in Figure 5.1(b) and Figure 5.6(a).

The asymmetry caused by a strip that is placed asymmetrically on the unit cell also depends on the thickness h of the strip and the difference between the refractive index of the strip n_{strip} and the other material covering the unit cell n_o (air, or an analyte in case of sensing), as illustrated by Figure 5.6(b) and (c). This is quantified by the optical asymmetry, α_{Optical} , which is the optical path length variation resulting from resonator illumination through the strip, normalized by $1 \mu\text{m}$ to arrive at a dimensionless parameter.

The area and optical asymmetries described above are general, applicable to any dielectric strip placed on any symmetric, planar resonator. However, there is also a unit-cell-specific contribution to asymmetry, α_{SRR} , as some areas of a resonator can be more sensitive to the presence of the strip than others. As illustrated by Figure 5.7, the SRR considered here is most sensitive to perturbations near the capacitive gap of the structure. Here we approximate this behaviour as linear, with α_{SRR} increasing from zero when the asymmetric strip area is centred infinitesimally close to the edge of the unit cell to two when the asymmetric strip area is centred infinitesimally close to the middle of the capacitive gap. This is quantified in terms of the distance $d_{x,\text{asym}}$ from the symmetry axis to the middle of the asymmetric strip area, and the lattice period P_x , see Figure 5.9(a). (If the strip covers the symmetry axis, $d_{x,\text{asym}} = (s_L + s_R)/2$, otherwise $d_{x,\text{asym}} = d_x$, where d_x is the distance of the centre of the strip from the symmetry axis.)

Figure 5.9(b), (c) and (d) show how the QBIC intensity, Q factor and FoM depend on the generalised asymmetry parameter, α . Various geometries were simulated to generate the figures, varying width, thickness and position of the Ge strip to modify the asymmetry as explained in the figure and its caption. For all cases, the QBIC intensity and Q factor follow an exponential trend as a function of asymmetry. The QBIC intensity increases exponentially, $I \approx 0.97 - 1.1 \exp(-0.46\alpha)$, and the Q factor decreases exponentially, $Q \approx 7 + 67 \exp(-0.84\alpha)$, as shown in Figure 5.9(b) and (c), respectively. Therefore, the FoM can be fitted with the product of these exponential fits, and the optimal asymmetry can be obtained from the saddle point of Figure 5.9(d). The optimal asymmetry of about $\alpha = 1.5$ corresponds, for example, to the half-Ge SRR sample with $h = 500$ nm. These results show how the asymmetry resulting from asymmetric placement of a dielectric strip on a symmetric unit cell can be quantified, and how this asymmetry is linked to the characteristics of the resulting QBIC resonance. By describing QBIC resonance intensity, Q factor and FoM as functions of all relevant physical characteristics of the strip (area, thickness, position and refractive index), we provide a solution for the inverse design of QBIC metamaterials, from desired resonance characteristics to physical parameters of the unit cell geometry.

Figure 5.9: Quantifying asymmetry and its effect on the QBIC resonance intensity, Q factor and Figure of Merit (FoM) based on simulations. (a) Asymmetry arising from width, translation and thickness of a dielectric strip is described by asymmetric parameters; α_{Area} , α_{SRR} and α_{Optical} . (b – d) Black circles represent the translation of 500-nm-thick Ge strips of either $s = 16 \mu\text{m}$ or $s = 47.5 \mu\text{m}$ width. Red crosses represent the thickness h variation of half-Ge strips ($s = 47.5 \mu\text{m}$) from 100 to 900 nm. Strip width s variation is represented by triangles and diamonds, where different symbols correspond to different Ge thicknesses as indicated and strips start from the centre and extend towards the left edge of the unit cell. Increasing and decreasing exponential functions fit the (a) QBIC intensity and (b) Q factor, and their product fits (c) FoM .

5.7 Conclusion

In summary, we demonstrated a novel class of active hybrid metamaterial devices and their inverse design. We showed how asymmetric placement of a semiconductor strip with nanoscale thickness on a symmetric resonator of substantially subwavelength size induces a quasi-bound state in the continuum resonance. Through photoexcitation of the semiconductor strips, we realized a narrow-band terahertz filter/modulator with 75% modulation and recovery time within 7 ps, exceeding modulation depth and switching speed of comparable silicon devices.^[21] Due to their high flexibility, our structures could be integrated into wearable devices. Our results indicate that the use of the area in between the semiconductor strips as microchannels for an analyte would result in a high-sensitivity refractive index sensor. By identifying the relationship of Q factor and intensity of the QBIC resonance with the unit cell's asymmetry, and expressing this asymmetry in terms of all relevant physical characteristics of the semiconducting or dielectric strip, we enable the inverse design of QBIC metamaterials. Our approach offers a possibility to functionalize any planar symmetric resonator that supports a BIC mode, to an active device with a high-quality factor. Thus, this work could lead to the functionalization of many existing metamaterial configurations, that are based on symmetric resonators to achieve switchable high Q resonances for the development and miniaturization of filters, modulators, and sensors.

5.8 Reference

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CHAPTER 6

Conclusion and Future Works

6.1 Conclusion

Metamaterial research continues to grow as it provides a platform for a myriad of fascinating applications such as spasers, perfect lenses, super oscillatory lenses, and perfect absorbers. In Chapter 1, we introduced the metamaterial platform and highlighted the lattice mode which is an inherent property that can be harnessed to improve metamaterial resonance response. The chapter also introduced bound states in the continuum which have become an interest to many scientists because of its theoretically infinite lifetimes and at its quasi-state possesses ultra-high Q factors. The chapter also listed several methods to functionalize metamaterial through external active perturbations: optical, thermal, and electrical. While chapter 2 discussed about the methods used to perform the experimental measurements.

Reducing losses and designing efficient metamaterial is very important for device integration such as spaser, narrowband filters, modulators, and sensors. Harnessing the diffractive losses from the periodic structures could reduce the loss and narrows metamaterial resonances. This diffractive loss, especially the 1st order, are trapped in the interface of the metal and dielectric layer. In chapter 3, we demonstrated that the lattice mode mediates the coupling between two of the constituent resonating arms of a split ring resonator in a unit cell. This mediative coupling splits and hybridized the resonance in the form of an anti-crossing (avoided crossing). This anti-crossing signifies a strongly coupled system and could be modelled with a classically coupled three oscillator model. In addition to the mediative coupling, the lattice mode frequency could be used to resonantly couple with each of the individual hybrid mode to achieve resonance narrowing and Q factor enhancement.

After verifying the role of the lattice mode in metamaterial. We investigate the lattice mode effect on a higher quality resonance such as the Fano resonance. Fano resonance or quasi-bound states in the continuum, possesses ultrahigh quality factor at low loss. Therefore, in chapter 4 we demonstrated the effects of lattice mode coupling to a Fano resonance engineered close to the lattice mode frequency. The design of the Fano resonance is done by changing the structural coupling of the split ring resonator from capacitive to inductive coupling. After the lattice mode couples to the Fano/QBIC resonance, we observed a significant enhancement in quality factor which brings the resonance closer to a bound state in the continuum while having its symmetry broken. Due to the radiative nature of metallic structures, lattice mode coupling provides a simple optimisation strategy to further enhance the Q factor of narrow resonance.

Other than breaking the symmetry of the resonators, in Chapter 5 we obtained a QBIC resonance by preserving structural symmetry of the resonator while breaking the out of plane symmetry by complementing the metamaterial structure with a nano-dielectric top layer. This nano-dielectric top layer covers half of the unit cell and half of the resonator, not only support the QBIC resonance but also supplements the resonance with photoactive modulation. The half covered dielectric layer could also be repurpose as microchannels which could be used for sensing. This strategy shown in this chapter could potentially be used on any symmetrical metamaterial to support a high Q resonance with photoactive modulation functionality. As such a general model was proposed to assist in the design of such hybrid structures with respect to its resonance intensity, Q factor and Figure of Merit.

In summary, our studies have shown a simple strategy for Q factor optimisation in metamaterials by utilizing its lattice mode. The lattice mode which is inherent in all periodic systems not only enhances the confined fields of resonating resonances but also mediates the coupling between constituent resonating components. We also proposed a new concept for

supporting a QBIC resonance in a symmetrical metamaterial for photoactive switching and sensing. We hope that our work can be a strategy used to design low loss and photoactive devices for future THz communications or applications.

6.2 Future works

Extraordinary transmission (ET) is mainly the cause of surface plasmon polariton (SPP) coupling on the interface of the periodic metal grating and dielectric. As mentioned in Chapter 1, the occurrence of the ET is strongly excited near the lattice modes as a resonant mode. Lattice modes or Rayleigh anomalies, on the other hand can be seen as non-resonant as they do not form a global maxima or minima in the far-field transmission but only a kink as seen in the chapters of the thesis. Another form of ET can be seen in guided mode resonance (GMR), which uses the lattice mode and total internal reflections to trap a leaky mode in the waveguide which re-radiates constructively in the far-field as a resonant mode. Exploiting the photoactive of semiconductors, we could modulate the amplitude of the ET resonance.

Other than symmetry protected bound states in the continuum, there exists another type of BIC which does not rely on the symmetry of the structure but the complete destructive interference of two coupled resonant modes, which is term the Friedrich-Wintgen BIC. We investigate other parameters to obtain a BIC while maintaining its structural symmetry. This can be done by exploiting phase changing materials such as superconductors, where its conductivity can be increased by cooling, in a metal superconductor hybrid system.

6.2.1 Dual Transmission Mode from Spoof Surface Plasmons and Localised Plasmons

As shown in Chapter 5, we demonstrated an active metamaterial device with a grating coupled to half a split ring resonator in a unit cell. Since it does not follow the conventional ET

equation, where a strongly excited resonant mode is located near the lattice mode in the x -polarization. More investigation needs to be done to discover the origin of this ET, but presumptions can be made that the ET resonance originates from the localized plasmons from the half SRR. Generally, this resonant feature can be induced through the inverse structure the SRR, i.e Babinet metamaterial, and have not been explored and reported in this configuration. This signifies that the grating lowers the background transmission and the SRR localized plasmons (LP) excites the transmission mode in the y -polarization and the aperture of the SRR excites spoof surface plasmons in the x -polarization.

The following investigation is to couple this LP resonance to the lattice mode of the system. Preliminary simulations reveal that by changing the length of the half resonator, we could tune the ET resonance close to the lattice mode and observe a resonance narrowing. The device shown in Figure 6.1 is optimised such that the resonance arises from the LP are close to the lattice mode, in contrast to the device in Chapter 5 there is a gap between the SRR and grating which lowers the resonance frequency significantly away from the lattice mode. Lossless simulations are done to investigate the possibility for the emergence of a BIC between the interference of the LP-ET and the lattice mode. However, the two modes, LP-ET and lattice mode, are of different type, one resonant in the far field while the other trapped in-plane of the device. As was highlighted by Sadrieva et al.^[1] that the lattice mode usually hinders structural eigen-resonance mode and is usually avoided in the investigation of BICs.

Figure 6.1: Simulated dual transmission mode arising from spoof surface plasmons and localized plasmons in the (a) x and (b) y polarization respectively.

6.2.2 Active Guided Mode Resonance

A grating metasurface can be used to diffract incident waves to the interface of the device but a waveguide obeying the conditions for total internal reflection can be used to couple and guide this diffracted wave. Because of the reciprocity of the grating, the guided waves can still leak out and constructively interfere in the form of a resonance in the far field. A square aluminium patch is used to support a polarisation independent GMR on a thin flexible substrate, Kapton. An additional active layer, Ge, is deposited in between the aluminium patch and substrate. This Ge interlayer functions as a screen which prevents the diffraction and modulates the GMR amplitude at higher conductivity, as shown in Figure 6.2.

The conditions for total internal reflections in a waveguide are given by $n_{\text{ext}} \leq n_{\text{wg}}$, where the n_{wg} and n_{ext} are the refractive index of the waveguide and external environment or cladding, respectively. Using the rigorous coupled wave theory, a guided wave can be excited in a waveguide grating if the effective refractive index of the grating, n_{eff} is between the external region and waveguide, $\max\{n_1, n_3\} \leq n_{\text{eff}} \leq n_{\text{wg}}$, where n_1, n_3 is the refractive index of the external environment, i.e if $n_1 = n_3 = n_{\text{ext}}$. n_{eff} can be obtained from the grating

equation, $n_{\text{eff}} = \left| n_1 \sin \theta_1 - m \lambda_0 / P \right|$. This device employs high amplitude and narrow band transmission which can be modulated for communications.

Figure 6.2: Simulation of an active guided mode resonance. (a) Metasurface schematic and (b) transmission with varying conductivity of Ge.

6.2.3 Conductance Bound States in the Continuum

This thesis mentioned the strategy to obtain bound states in continuum with metamaterial resonators and access to high Q resonances by breaking its symmetry. Another class of BIC is observed by preserving the metamaterial symmetry but changing the material or conductivity of the constituent resonating arms. In Figure 6.3, the left resonating arm is constituted of aluminium and the right is YBCO at 100 nm. YBCO is a superconducting material with a superconducting phase transition at 85.1 K for a 100 nm thick film. In part (a) of the same figure, a Fano resonance arises as the YBCO is at its superconducting state, 20 K, while maintaining symmetry. In Figure 6.3(b), the symmetry is broken by shifting the gaps by displacement, d . At negative displacement d , the superconducting resonating arm constitutes the majority of the SRR while at positive displacement d , aluminium is the majority. Notably at $d = 3 \mu\text{m}$, the Fano resonance vanishes and emerges as d is increased further. This hints that the conductance, $G \propto \sigma/L$, plays a part in decoupling and coupling this hidden mode from the continuum, where σ is the conductivity and L is the length of the resonator. Similarly, in (a),

at its superconducting state, the conductivity of YBCO is significantly larger than aluminium causing a difference in the coupling of the two-constituent resonating arm and a Fano resonance. More need to be done to verify if this Fano resonance arises from bound states in the continuum. This opens avenues to explore to obtain Fano resonance without constraining to structural parameters.

Figure 6.3: Simulations of superconductor metal (YBCO-Al) hybrid system. (a) Transmission of device in a symmetric configuration ($d = 0 \mu\text{m}$) at 20 K and 100K. (b) Transmission of device in an asymmetric configuration with increasing d at 20 K.

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