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High- Q lattice mode matched structural resonances in terahertz metasurfaces

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The quality (Q) factor of metamaterial resonances is limited by the radiative and non-radiative losses. At terahertz frequencies, the dominant loss channel is radiative in nature since the non-radiative losses are low due to high conductivity of metals. Radiative losses could be suppressed by engineering the meta-atom structure. However, such suppression usually occurs at the fundamental resonance mode which is typically a closed mode resonance such as an inductive-capacitive resonance or a Fano resonance. Here, we report an order of magnitude enhancement in Q factor of all the structural eigenresonances of a split-ring resonator fueled by the *lattice mode matching*. We match the fundamental order diffractive mode to each of the odd and even eigenresonances, thus leading to a tremendous line-narrowing of all the resonances. Such precise tailoring and control of the structural resonances in a metasurface lattice could have potential applications in low-loss devices, sensing, and design of high- Q metamaterial cavities. *Published by AIP Publishing.*
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The collective response of meta-atoms in a lattice determines the effective properties of the metamaterial medium.¹ The radiative behavior is also an outcome of the interactions among the unit cells in the lattice. However, recent demonstrations reveal that the lattice mode mediates the interaction between the meta-atoms and such interactions lead to the excitation of extremely sharp resonances in metamaterial and plasmonic systems.^{2–10} Sharp resonances are desirable for multifunctional applications in sensing, enhanced light-matter interactions, non-linearity, and design of efficient cavities for lasing applications.^{11–18} Therefore, lattice modes provide a rather straightforward route to excite high Q factor resonances in an otherwise lossy system, where the linewidth of the plasmonic and metamaterial resonators are limited by the material conductivity and subwavelength nature of the resonators.¹⁹

In this Letter, we strategically match the lattice mode to each of the odd and even eigenresonances of a split-ring resonator (SRR) meta-atom. Previous works on lattice mode matching (LMM) with the eigenresonance of a plasmonic or a metamaterial resonator have been restricted to the resonance line-narrowing and Q factor enhancement of just one of the many eigenmodes of the resonator.^{6,20} Therefore, we performed a detailed investigation on the lattice mode-matching with each of the different odd and even eigenresonances of the SRR. Through detailed experiments and numerical calculations, we show that all the eigenmode resonances of a SRR undergo tremendous sharpening of the resonance linewidth as the lattice mode approaches the resonance frequency of a specific odd or even eigenmode resonance. We found that the fundamental lattice mode could enhance the Q factor of all the SRR resonances by nearly an order of magnitude. Such

a dramatic enhancement in the Q factor of metamaterial resonances addresses the problem of radiative loss to a large extent and thus could have many device applications, including narrowband filters and terahertz sensors.^{21–23}

The design and dimensions of the SRRs are illustrated in Fig. 1. The square SRR has a length of $36\ \mu\text{m}$ with an arm-width of $6\ \mu\text{m}$ and a split gap of $3\ \mu\text{m}$. The metasurface samples are fabricated on an n-type $640\text{-}\mu\text{m}$ thick silicon substrate by conventional photolithography technique. The 200-nm thick aluminum film is uniformly deposited by thermal evaporation. In order to study the effect of the lattice modes, several metamaterial samples with lattice constants varying from 40 to $200\ \mu\text{m}$ were fabricated, as shown by microscopic images in the inset of Fig. 1. A photoconductive

FIG. 1. Microscopic images of metasurface samples. Dimensions of the square split-ring resonator are $36\ \mu\text{m}$, $w = 6\ \mu\text{m}$, and $g = 3\ \mu\text{m}$. For the fixed-size resonator, the lattice constant is varied between 40 and $180\ \mu\text{m}$, as shown in the insets.

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switch based $8f$ confocal terahertz time-domain spectroscopy was used to characterize the transmitted dispersion properties of the metasurface.²⁴ With the terahertz beam illuminating the sample at normal incidence, the transmission at both the polarizations, namely, the electric fields polarized parallel and perpendicular to the gap (y and x axes in Fig. 1) are recorded. The electric field in the y -direction excites the odd modes ($n = 1, 3$), and the field in the x -direction excites the even mode ($n = 2$) of the SRR.²⁵ The beam waist diameter of the $8f$ confocal system illuminating the metasurface sample is 3.5 mm. The transmission amplitude is calculated as $t(\omega) = |E_s(\omega)/E_r(\omega)|$, where $E_s(\omega)$ and $E_r(\omega)$ are the Fourier transforms of the transmitted signals through the sample and the reference, respectively. A blank silicon wafer identical to the metamaterial substrate is used as a reference. The spectral resolution of the measurement is 59 GHz by carrying out 17 ps time-domain terahertz pulse scan.

We designed the experiment by performing extensive simulations using CST Microwave Studio solver. Based on the finite-difference time-domain (FDTD) method, the transmission amplitude is simulated by the frequency-domain solver with the unit cell boundary condition that has 5 GHz spectral resolution. The permittivity of the silicon substrate and the conductivity of aluminum used in the simulation are $\epsilon = 11.96 + 0.05i$ and $\sigma = 3.72 \times 10^7$ S/m, respectively. With the electric field parallel to the gap of SRRs (y -direction), the odd resonance modes $n = 1$ and $n = 3$ are excited, as shown by the blue rectangular region in the simulated transmission in Fig. 2(a). The colors in the map indicate the transmission amplitude strength, where the x -axis denotes the frequency and the y -axis represents the change in the lattice constant or periodicity. At around 0.5 THz, the inductive-capacitive (LC) mode ($n = 1$) gradually becomes narrower in resonance linewidth with increasing periodicity. The same behavior is observed for the quadrupole mode ($n = 3$) at around 1.5 THz. Both of these odd resonance modes show significant line-narrowing at different lattice constants of 180 and 60 μm , respectively. This occurs due to

the alignment of the fundamental order diffractive (from lattice) mode with each of the individual resonance modes. For the $n = 1$ mode (LC resonance), the metasurface lattice constant of 180 μm supports the fundamental order diffracted light that has identical frequency as the LC resonance. Similarly, for the $n = 3$ mode (quadrupole), a lattice constant of 60 μm causes line narrowing of the quadrupole resonance mode.

In a square array with period P , the lattice modes excited at different frequencies obey the following relationship:

$$f^2 = \left(\frac{c}{n_s P}\right)^2 \times (i^2 + j^2), \quad (1)$$

where f is the frequency of the diffracted lattice mode, n_s is the refractive index of the substrate, and c denotes the speed of light in vacuum. The integer pair (i, j) specifies the order of the diffraction mode. We match only the first order (1,0) or (0,1) diffraction mode since this is the mode that has the maximum intensity of the trapped light in the metasurface plane.⁶ Thus, the periodicity versus frequency relationship for the first order diffraction mode (1,0) or (0,1) can be further simplified to

$$f = \frac{c}{n_s P}, \quad (2)$$

which is plotted (solid curve) in Fig. 2 with varying lattice constant on the y -axis and frequency on the x -axis. We define the intersection of the first order diffracted mode and the eigenresonance frequency of the SRRs as the *critical periodicity*, P_c . Therefore, the lattice constant of a SRR array has three different critical periodicities, $P = P_{c1}, P_{c2}$, and P_{c3} , that correspond to the first three eigenmode resonances ($n = 1, 2, 3$) of the chosen SRR design. Thus, for the y -polarized terahertz wave incidence, $P_{c1} = 180 \mu\text{m}$ and $P_{c3} = 60 \mu\text{m}$ denoting the critical periodicities for the $n = 1$ and $n = 3$ modes as indicated by the dashed horizontal lines (parallel to the x -axis) in Fig. 2(a). The higher resonance frequency of the quadrupole mode ($n = 3$) shrinks the critical periodicity compared to the LC mode ($n = 1$) which is at a lower frequency. The even $n = 2$ mode has a dipolar characteristic which is excited with the terahertz field polarized along the x -direction as labelled in Figs. 2(b) and 2(d) which shows the simulated and the measured results. Here, the diffractive mode matching occurs at the critical period of $P_{c2} = 80 \mu\text{m}$. We note that the dipolar mode is extremely broad at $P = 40 \mu\text{m}$. However, it undergoes a sudden line-narrowing when it approaches the critical periodicity of 80 μm . Thus, we note that by varying the lattice constant, the diffraction mediated coupling in a metasurface array leads to a tremendous sharpening of all the SRR structural ($n = 1, 2, 3$) resonance modes. We also notice frequency blue shift of all the three resonance modes in Figs. 2(a) and 2(b) as the periodicity is reduced by bringing the SRRs closer to each other. The near-field inductive coupling leads to cancellation of the mutual inductance which reduces the net inductance in the nearest neighbor coupled system, and thus, the fundamental LC resonance shifts to higher frequency since the resonance $f_0 \propto 1/(\text{LC})^{1/2}$. Once the fundamental resonance blue shifts, all its harmonics also shifts to higher frequencies due

FIG. 2. (a) Simulated and (c) measured transmission map for the LC ($n = 1$) and quadrupole modes ($n = 3$) with varying lattice constant for the y -direction E field incidence. (b) Simulated and (d) measured map for the dipole mode ($n = 2$) versus lattice constant for the x -direction E field incidence. The solid curves show the variation of the first order diffraction mode (0,1) while the critical periodicity P_{c1} , P_{c2} , and P_{c3} are indicated by the horizontal dashed lines.

to the nearest neighbor interaction in the metamaterial lattice. The measured transmission spectra in Figs. 2(c) and 2(d) are consistent with the simulation results. The disagreement between simulation and measurements at the LC resonance ($n=1$) mode is due to the limited spectral resolution of our measurements.

Figures 3(a)–3(c) show the simulated normalized transmission amplitudes of all the odd and even eigenresonance modes ($n=1, 2, 3$) of the SRR with varying lattice constants. Since the critical periodicity for the $n=1$ mode is $P_{c1}=180\text{ }\mu\text{m}$, we observe that as we increase the lattice constant to approach this critical period, the LC resonance gradually narrows down and becomes extremely sharp. Beyond the critical period, we observe a sudden broadening of the resonance. The Q factor at the critical lattice constant is enhanced by fifteen-fold compared to that at mismatched lattice constant of $40\text{ }\mu\text{m}$. The $n=2$ eigenmode, which is the dipole resonance undergoes resonance line-narrowing with the increase in the lattice constant from $40\text{ }\mu\text{m}$ to the critical periodicity $P_{c2}=80\text{ }\mu\text{m}$. Beyond P_{c2} , the linewidth broadens even for a small increase in the lattice constant to $90\text{ }\mu\text{m}$, which highlights that even minor mismatch in the lattice constant would lead to large broadening of the structural eigenresonance. We also observed the resonance linewidth tailoring of the $n=3$ quadrupole mode where the linewidth shrinks as the critical periodicity is approached followed by a broadening as the lattice constant was further expanded beyond the critical periodicity. This precise tailoring of the Q factor of all structural resonances in an SRR array shows that the *lattice mode matching* (LMM) could be one of the most straightforward and efficient way to suppress or tailor the radiative loss in metamaterial and plasmonic systems. This finding is essential since the radiative loss channel cannot be tuned to such a large extent by altering the material properties or the shape of the resonators. Another remarkable observation is that even the highly radiative resonances such as the dipole and the quadrupole modes here ($n=2, 3$) undergo huge enhancement in their Q factors which is nearly six to seven-fold ($Q=1.0$ to 6.2 for $n=2$ and $Q=2.4$ to 19.6 for $n=3$). Figs. 3(d)–3(f) present the measured resonance lineshape of

FIG. 3. Normalized simulated (a)–(c) and measured (d)–(f) spectra that have been aligned to match the resonance transmission minimum of each curve with varying periodicities for the $n=1$, $n=2$, and $n=3$ modes. We align the transmission minima to highlight the resonance linewidth broadening at the same frequency, therefore ignoring the frequency shifts due to near field coupling effects.

each mode. The extracted Q factors from the measurement of the $n=2, 3$ modes agree reasonably well with the simulation results while the disagreement of $n=1$ is caused by the low frequency resolution of the time-domain scan which is limited due to the Fabry-Perot reflections from the rear surface of the metasurface substrate. The spectral resolution between simulations and measurements shows nearly an order of magnitude difference and the resonance line-narrowing effect cannot be captured in the measurements if the linewidth is much smaller than the spectral resolution. In our case, the measured spectra could resolve the $n=2, 3$ modes which are much broader in linewidth compared to the $n=1$ mode whose lattice matched linewidth is reduced to 12 GHz , which is significantly smaller than our measurement resolution of 59 GHz . Thus, using the high resolution (5 GHz) numerical solver, we could accurately extract the linewidths of all the eigenresonances, where the agreement between simulations and measurements were found to be good for the $n=2, 3$ modes.²⁶

Tailoring of the Q factor due to variations in the lattice constant is plotted in Figs. 4(a)–4(c) for each eigenmode ($n=1, 2, 3$). At the $n=1$ LC mode, the Q factor is 2.2 at $40\text{ }\mu\text{m}$ and gradually increases to 25.8 at $160\text{ }\mu\text{m}$, then rises steeply to 34.3 at the critical periodicity $P_{c1}=180\text{ }\mu\text{m}$. With a further increase in the lattice constant, the mismatch of the fundamental order diffractive lattice mode leads to a sudden drop in the Q factor to 14.7 . A similar trend is observed for the $n=3$ mode, where the lattice constant variation from 40 to $50\text{ }\mu\text{m}$ results in an increase of the Q factor from 2.4 to 5.1 . However, when the lattice constant is further increased to the critical periodicity $P_{c3}=60\text{ }\mu\text{m}$, we notice a sharp enhancement in the Q factor to 19.6 and then it declines suddenly to 3.8 when the lattice constant is further increased to $70\text{ }\mu\text{m}$. Although being restricted by the high radiative loss nature of the dipole $n=2$ mode, a similar trend in the Q factor variation is noticed when the lattice constant gradually approaches and then deviates from the critical period $P_{c2}=80\text{ }\mu\text{m}$. For all the eigenmodes, it is worth noting that the Q factor increases gradually when the lattice constant approaches the respective critical periodicities and then it declines drastically beyond the critical periodicities due to the lattice mode mismatch. From the perspective of near-field coupling in a metamolecule array the separation between the unit cells determines the collective behavior.¹ The increase in lattice constant could reduce the damping loss by isolating the nearest neighbor meta-atom.^{27,28} Here, we demonstrate the line narrowing of all the structural eigenmodes which are the harmonics of the fundamental ($n=1$) mode and observed that the Q factor

FIG. 4. Extracted Q factors of (a) LC ($n=1$), (b) dipole ($n=2$), and (c) quadrupole ($n=3$) modes with varying periodicities. The polarization of the terahertz field is indicated in the inset. The critical periodicities are indicated by the dashed lines.

could be enhanced for any metamaterial resonance as long as the resonance wavelength matches the fundamental lattice mode which we define here as the *lattice mode matching* (LMM) phenomena. Since a single-split ring resonator is one of the simplest cases of a metamaterial resonator, we believe that the Q factor enhancement upon LMM is a universal phenomenon and would occur for any structural metamaterial design across the electromagnetic spectrum.

In order to elucidate the underlying mechanism of the sharp enhancement in the Q factor of the eigenmodes through LMM, we performed numerical simulations to closely explore the confined electric field and the surface currents in the SRR structure. The electric field and surface current distributions for each resonance mode at critical period and off-critical period are shown in Figs. 5(a), 5(c), and 5(b), 5(d), respectively. The critical periodicities for different order resonances $n = 1, 2, 3$ are $P_{c1,2,3} = 180, 80,$ and $60 \mu\text{m}$, respectively, while we chose the off-critical period as $40 \mu\text{m}$ for all the modes to observe a large impact of the LMM phenomena. For the $n = 1$ LC resonance which is lattice matched to the lattice mode, we observe the electric field to be tightly confined in the SRR gap which shows a stronger confinement than that in the mismatched case. Rows 2 and 3 in Fig. 5 show the electric field at the modes $n = 2, 3$ which corresponds to the dipole and quadrupole features, respectively. Even in these two cases, we observe strong electric field distribution concentrated in the SRR structure. A tremendous field enhancement at all resonance modes is verified for the lattice-matched case compared to that of the mis-matched case. The tight field confinement manifests an extremely low radiation loss in all the resonance modes, which is due to trapping of the diffracted light in the metasurface lattice. When the lattice mode is matched to the structural resonance, the incident field is coupled to the resonators via constructive interference of the scattered fields from the meta-atom and the periodic lattice.^{29,30} Such strong coupling between the lattice mode and metamaterial resonance modes leads to suppression of the radiative loss, which gives rise to a sharp enhancement in the Q factor, irrespective of the nature of the metamaterial structural resonance mode. Accordingly, the surface currents

in Fig. 5(c) are pronouncedly dense and strong compared to that of the mismatched diffraction mode case, as shown in Fig. 5(d). For the mismatched-lattice mode case, the scattered fields radiate out into the free space, giving rise to a broad resonance due to high radiative loss. Therefore, by merely varying the lattice constant of the arrays, we can engineer the radiation characteristic of all the eigenresonance modes in a metamaterial and plasmonic system from being super-radiative to sub-radiative.

In summary, we demonstrate that *lattice mode matching* leads to nearly an order of magnitude enhancement in the Q factor of all the structural resonances in a metasurface array. The fundamental order diffractive lattice mode traps the electromagnetic fields in the lattice plane and constructively interferes with the structural resonances irrespective of the nature of each individual eigenresonance. Such a straightforward strategy to enhance the resonance modes of a metamaterial array could lead to efficient design of low-loss metadevices. The high Q factors could be exploited for sensing, narrow-band filtering, and laser spasing applications across different electromagnetic domains, including the terahertz frequency regime.

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FIG. 5. (a) Electric fields and (c) surface currents for the diffractive mode at the LC ($n = 1$), dipole ($n = 2$), and quadrupole modes ($n = 3$) with corresponding lattice constants of 180, 80, and $60 \mu\text{m}$. (b) Electric fields and (d) surface currents for the mismatched lattice constant of $40 \mu\text{m}$ at the LC ($n = 1$), dipole ($n = 2$), and quadrupole ($n = 3$) resonance modes.

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