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Near-field investigation of the effect of the array edge on the resonance of loop frequency selective surface elements at mid-infrared wavelengths

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Abstract: Mid-infrared scattering scanning near-field optical microscopy, in combination with far-field infrared spectroscopy, and simulations, was employed to investigate the effect of mutual-element coupling towards the edge of arrays of loop elements acting as frequency selective surfaces (FSSs). Two different square loop arrays on ZnS over a ground plane, resonant at 10.3 µm, were investigated. One array had elements that were closely spaced while the other array had elements with greater inter-element spacing. In addition to the dipolar resonance, we observed a new emergent resonance associated with the edge of the closely-spaced array as a finite size effect, due to the broken translational invariance.

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subwavelength elements or apertures arranged in a periodic pattern across a surface in an array and can be used to tune a range of properties such as absorptivity/emissivity, reflectivity, transmission, polarization, beam shape, etc [7–9]. Many designs are based on arrays of metallic elements where the resonances can be tuned to different wavelengths by changing the geometric dimensions of the individual elements and/or other features of the design. Evanescent electric-field coupling among neighboring FSS elements, which is affected by the inter-element spacing, has been found to be an important factor in determining the resonant properties of such structures and, consequently, the spectral response [10–13].

Much of these properties of FSSs are dictated by the near-field response, which can be measured using scattering-type scanning near-field optical microscopy (s-SNOM) [10,12,14–21]. Previously, we investigated the near- and far-field response of semi-infinite arrays composed of two different size square loops [12]. The amplitude and phase of the near-field measurements show that these strongly absorptive structures support fundamental (dipolar) and second harmonic (quadrupolar) resonance modes when illuminated with 10.6 µm wavelength monochromatic radiation at 60° off-normal angle of incidence.

Practically, these arrays of elements have finite sizes that depend on the application and fabrication restrictions. However, they are usually modeled as infinite arrays for predicting their electromagnetic response [22]. This approximation is typically sufficient for the design of these structures when the fabricated array will be relatively large, but the actual electromagnetic response of the array will deviate more from the simulated response as it becomes further truncated [23]. This has been shown previously for smaller arrays designed for RF frequencies [22,24–26]. More recently, the effect of truncation has been shown at infrared wavelengths using near and far-field measurements [15]. In this work we showed that truncation of square loop arrays caused the resonance to blue shift. However, the measured near-field response was difficult to interpret mainly due to the effect of truncation in two dimensions, which complicates the inter-element coupling, especially for the smaller truncated arrays. However, it was apparent that there was less uniformity in the near-field response across each of the elements when the arrays were decreased in size. Overall, it was concluded that the blue shift of the spectral response of these truncated arrays was due to the diminished amount of nearest and next-nearest neighbor coupling among the elements as the arrays became smaller. A blue shifting response caused by decreased inter-element coupling has been shown for nanoparticle arrays and dimer antennas as well [27–30]. Interestingly, these results suggested that for much larger arrays, the local resonant wavelength among the elements would gradually shift to shorter wavelengths towards the edge, which inspired this work.

In this work we explore the effect of coupling on the resonant properties for arrays of different size loop structures on ZnS having different inter-element spacing, especially towards the edge of the arrays. For the two arrays of different inter-element spacing, the resonant wavelength was matched by adjusting the loop size. The study of near- and far-field responses towards the edge of these arrays reveals the appearance of a new resonance feature due to the truncation.

2. Materials and methods

2.1 Simulations and fabrication

It was of interest to explore the resonances at the edge of arrays of metallic elements on a dielectric layer without loss bands in the spectral region where the dipolar resonance for the elements is located. ZnS has loss bands far removed from ~10 µm wavelength, which is the spectral region of interest and, thus, avoids potential coupling or overlap between the array and material resonances that has been observed in previous work [12,30].

The design consisted of arrays of two different size square loops on ZnS having different inter-element spacing, which were both designed to have a peak resonance under s-polarized
transverse electric), 10.25 µm wavelength illumination at 60° off-normal angle of incidence. Finite element method commercial software, Ansys HFSS, was used to optimize the designs for illumination at this polarization, wavelength, and angle of incidence. Frequency dependent optical constants for all materials used in the designs were determined by ellipsometry and employed in the simulations. Floquet port analysis was used to excite a unit cell of the structures with an s-polarized beam where periodic boundary conditions were applied on adjacent faces of the model to represent a repeating infinite array. Absorptivity and relative phase change upon reflection of the reflected radiation were determined from the s-parameters derived from the Floquet port analysis. Also, local electric field values were obtained from the same simulations.

Based on these simulated results, the fabrication was completed to make the two arrays of loops over a chromium ground plane with a ZnS spacer layer, which was performed using a similar procedure as to what is described in a previous report [15]. Cr was employed as the ground plane due to the relatively good adhesion between Cr and ZnS. Briefly, a 150 nm Cr ground plane was deposited by e-beam onto a freshly cleaned silicon wafer. Next, 0.32 µm of ZnS was deposited by thermal evaporation using a baffled box, which allowed for more control in the deposition process and improved uniformity in the resulting film. The loop structures were patterned in a film of polymethyl methacrylate (PMMA) resist using e-beam lithography, which was followed by metallization with 2.5 nm of titanium and 75 nm of gold. Lift-off was facilitated by submerging the sample in n-methyl pyrrolidinone (NMP). The resulting loop structures are shown in the scanning electron micrographs in Figs. 1(a) and 1(b).

2.2 Near-field characterization

Near-field measurements were performed with a custom built s-SNOM, which has been described in previous works and is shown in the schematic in Fig. 2 [12,15]. Briefly, a CO₂ laser (L4S, Access Laser Company) operating at 10.25 µm is employed as the source. In the configuration for this setup the incident beam is directed towards a beam splitter (BS) where a fraction of the beam is reflected towards the sample and a comparable fraction is transmitted through into a reference path. The reflected beam is then focused using an off-axis parabolic (OAP) reflector to a diffraction limited spot onto the sample at 60° off-normal relative to the surface plane. The AFM tip, which is operating in tapping mode at a frequency of 240-280 kHz, scatters the exited near-field and the scattered light is collected with the same set of optics as was used for the incident beam (reflection-mode backscattering configuration) [31]. The portion of the incident beam transmitted into the reference path then passes through a quarter wave plate (QWP) and is reflected off of a moveable mirror (MM), which rotates the polarization of the beam and effectively allows for attenuation of the reference power. Both beams are recombined at the BS in a Michelson configuration, then focused onto a mercury cadmium telluride (MCT) detector. The following equation can be used to define the intensity of the signal (S_d) at the detector:

![Fig. 1. SEM micrographs of (a) the smaller, closely-spaced loops on ZnS, and (b) the larger, more widely spaced loops on ZnS.](image-url)
where $E_{\text{scat}}$ is the electric field of the scattered beam, $E_{\text{ref}}$ is the electric field of the reference, $I_b$ is background signal not originating from the near-field signal, and $\phi$ represents the relative phase difference between the reference and the scattered beam [31,32]. The well-established cross polarization-detection scheme for s-SNOM is employed to limit background signal [16,18,33,34]. Here, the sample is excited with s-polarized light while the tip is predominantly scattering off p-polarized light, which is what is measured at the detector and is proportional to $E_z$. In addition, a lock-in amplifier was used to extract the signal at the second harmonic of the AFM tip vibrational frequency ($\Omega$), which further suppresses unwanted background.

![Fig. 2. Schematic of the s-SNOM setup operating at a wavelength of 10.25 µm and based on a tapping mode AFM.](image)

**2.3 Far-field characterization**

Far-field spectral measurements were performed using a Perkin Elmer FT-IR microscope. A variable size aperture was used to restrict the measurement to very small areas of the arrays being measured. Using an in-line optical microscope, the sample was translated on the microscope stage to different positions to allow for different locations near the edge of the arrays to be measured, which allowed for spatially resolved spectra to be obtained. The angle of illumination was predominantly normal to the surface plane. Due to the diminished signal when using small apertures, the measurements had to be taken with unpolarized light. Since the presence of an optically thick ground plane effectively prevents any transmission, absorptivity was calculated from the measured reflectivity by: absorptivity = 1−reflectivity.

**3. Results**

**3.1 Design simulations**

Two different designs of square loop arrays on ZnS were optimized through parametric simulations: arrays of closely-spaced loops and arrays of loops with larger spacing. Plots of
absorptance and reflected phase versus element size are useful for determining the resonant dimensions of elements designed for a particular wavelength and angle of illumination, especially in designing reflectarrays [21,35–37]. Here, one design was intended to be composed of square loop elements having a small periodicity and larger inter-element coupling while the other design was composed of square loop elements having a large periodicity and minimal inter-element coupling. The square loop array having a large periodicity was designed to effectively be a single element array and act as a control experiment.

Therefore, parametric simulations were performed where infinite arrays of square, Au loop elements having a range of sizes and a periodicity of 1.79 µm were illuminated with incident radiation having a wavelength of 10.25 µm and an angle of incidence of 60° off-normal using a Floquet port. Then, similar simulations were performed under the same conditions, except with the loop elements having a periodicity of 10 µm. Results for these simulations are shown in Fig. 3(a) where the absorptance from the loop elements having a periodicity of 1.79 µm are represented by the blue dashed line while the loop elements having a periodicity of 10 µm are represented by the black dotted line. The graph shows that smaller spacing between the elements in the array requires the element size to be smaller in order to maintain the same peak wavelength of resonance. Presumably, the shifting of the peak wavelength of resonance for different periodicities is due to coupling among the elements, which has been shown in the literature for other types of elements such as square loops and end-loaded crosses [10–12]. To confirm that the 10 µm period loop arrays were effectively behaving as a single element array and to determine the periodicity at which coupling among the elements is removed, the previous simulations were also performed at a range of different inter-element spacing. As before, the arrays were illuminated with incident radiation having a wavelength of 10.25 µm and an angle of incidence of 60° off-normal using a Floquet port. Results for this set of simulations is shown in Fig. 3(b) where the resonant size of the loop is plotted as a function of the periodicity. It can be observed that as the periodicity approaches 10 µm there is very minimal change in the resonant edge length for the loop structures. Based on these results, two arrays having different size loop elements and inter-element spacing were fabricated. The arrays of closely-spaced loops were fabricated with a loop edge length of 1.39 µm and periodicity of 1.79 µm. The arrays of loops with greater inter-element spacing had a loop edge length of 1.6 µm and periodicity of 10 µm.

Fig. 3. Simulated (a) absorptance versus edge length for loops of 1.79 µm (blue dashed line) and 10 µm (black dotted line) periodicity when the structures were illuminated with a 10.25 µm wavelength incident wave 60° off-normal to the surface plane. Simulated (b) resonant edge length versus periodicity (blue dash-dot line) when the structures were illuminated under the same conditions as in (a). There is a shift in the resonant size to large loop sizes as the periodicity is increased until about 2.5 µm periodicity and the plot suggests that at near 10 µm periodicity there is minimal effect of periodicity on the resonance.
3.2 *Far-field FT-IR*

First, as described previously, FT-IR spectra were taken locally around the edge of the loop elements on ZnS having different inter-element spacing. The measurements were performed with the variable size aperture for the FT-IR microscope adjusted to be as small as possible, but still large enough to obtain a measurable, clear signal. Unfortunately, measurable signal could not be obtained for individual loops by making the aperture smaller. So, for the closely-spaced loops the variable aperture was set to be very large in the dimension along the edge of the array and to ~21 µm in the other dimension, which is nearly equal in size to an area of twelve columns of loops. For the loops with larger spacing, the variable aperture was set to be very large in the dimension along the edge of the array and to ~33 µm in the other dimension, which covers an area equal in size to three columns of loops.

Due to difficulties in simulating the experimental measurement where the array is excited over a relatively small, finite area including areas with and without elements, the simulated local absorptivity over several unit cells and across areas around the array could not be accurately determined. Therefore, in the simulation the whole array was excited, but the averaged power loss was calculated over close to the same area as was measured in the experiment. These values were determined by integrating the volume loss density over the volumes in each of the unit cells in this area to yield absorbed power loss.

![Fig. 4. Measured spectral absorptivity and simulated power loss towards the edge of the array of closely-spaced loop elements on ZnS. The experimental results were obtained by FT-IR and the simulated results were obtained by integrating the volume loss density over the same spectral range. The experimental and simulated data were both obtained at normal incidence. The inset shows a graph of experimental and simulated peak wavelength as a function of position towards the edge of the array, which was derived from the experimental and simulated spectra.](image)

Figure 4 shows the spectral absorptivity towards the edge of the array of closely-spaced loop elements on ZnS compared to simulations of the power loss over the same spectral region and location along the edge of the array. Here, for the measured result, the sample was positioned relative to the aperture so the first three columns of elements were measured, the first six were measured, the first nine were measured, and the first twelve were measured. In
addition, measurements were made in the center of the array at a relatively large distance from the edge. It should be noted that in most of the measurements performed there were areas void of any loops that contributed to the measurements, except for when the first twelve columns of elements from the edge was measured and when the measurement towards the center of the array was performed. Therefore, the absorptivity in the spectra is shown to be diminished for measurements done towards the edge of the array, which can be attributed to decreased fill factor where more of the measured area includes areas void of any elements. Also, in the spectra of the measured absorptivity and simulated power loss there is a blue-shift in the peak resonance position for the loops towards the edge of the array. This trend is shown more clearly in the inset in Fig. 4, which is a plot of the peak wavelength position from the simulated and experimental results as a function of position towards the edge of the array. The simulated results show a qualitative match with the experimental result where differences can be attributed to the difficulties in replicating in the simulation how the measurement was performed.

In comparison, as a control measurement, FT-IR measurements at the edge of the square loop arrays with greater inter-element spacing showed no observable blue-shifting of the peak resonance position as the aperture was moved from the center of the array towards the edge. This was expected and illustrates how important inter-element coupling is in determining the properties of arrays, especially at the edge.

3.3 Near-field NSOM

Next, near-field measurements were taken locally around the edge of the arrays of closely-spaced loop structures on ZnS. Figure 5 shows experimental and simulated near-field images of the closely-spaced loop elements at the edge of the array where the edge of the array is on the right side of the image (as indicated by the arrows). The experimental amplitude image (Fig. 5(a)) clearly show a strong dipolar (fundamental) resonance for the elements towards the center of the array where there is a qualitative match between the simulations and experimental data. Similarly, the experimental and simulated phase images shows a 180° phase shift across the elements (Figs. 5(b) and 5(d)), which is consistent with the presence of a dipolar mode. However, there is asymmetry in the amplitude values across many of the elements. More interestingly, the amplitude shows strong variations towards the edge of the array and shows a stronger response over some of the elements within a couple columns from the edge of the array. The phase shows similar variations as well. In order to examine the amplitude and phase variations in these images, a line scan analysis of these images was done across the elements approaching the edge of the array. Figure 6(a) shows experimentally (black square points) and simulation (red circular points) derived plots of the average near-field amplitude as a function of element number (where “1” is the element at the edge of the array as indicated by the arrow). Figure 6(b) shows experimentally (black square points) and simulation (red circular points) derived plots of the average near-field phase as a function of element number. A plot of the moving average of the experimental data is shown in both Figs. 6(a) and 6(b) as a guide to the eye. Here, one can more clearly see that the near-field amplitude and phase varies across the elements near the edge of the array for both the measurement and simulations. There is good agreement between the simulated and experimental near-field phase in Fig. 6(b), but the simulated near-field amplitude varies more significantly than the experimental amplitude in Fig. 6(a). Previously, it was shown that the experimental and simulated near-field amplitude varied to different extents from column to column among elements in truncated arrays of loops [15]. The differences in the variations for the simulations and experimental data was partly attributed to differences in the geometry of the fabricated and simulated structure where in the fabricated structure there is more significant roughness and curvature along the edges. Similarly, we attribute the differences in the amount of amplitude variation across the loops to differences in the geometry between simulated and experimental results.
Fig. 5. Measured (a, b) and simulated (c, d) near-field images near the edge of the array composed of the closely-spaced loop elements on ZnS. Specifically, this array had a periodicity of 1.79 µm. In these images the elements at the edge of the array are on the right side of the images as indicated by the arrows. In the measured amplitude images the values for the z-axis, represented by the color bar, are proportional to $E_z$.

Fig. 6. Graphs of (a) simulated (red circular points) and experimental (black square points) near-field amplitude versus element number and (b) simulated (red circular points) and experimental (black square points) near-field phase versus element number for the closely-spaced loop elements on ZnS where element “1” is the element at the edge of the array as indicated by the arrows. The above values were determined by line scan analysis that was performed across a row of elements in the images in Fig. 5. The average value for each quantity was calculated over each element to yield the above values. The red lines are present as a guide to the eye and are the result of a moving average applied to the points.

For comparison, the above near-field measurements were repeated with the square loop arrays on ZnS with greater inter-element spacing (not shown). In contrast to the closely-
spaced loops, each element showed a more symmetric dipolar response in the amplitude image. Also, the amplitude did not vary significantly across the columns of elements. The near-field phase remained nearly constant across the elements around the edge of the array.

4. Discussion

Therefore, the closely-spaced loops on ZnS show a stronger edge effect compared to the loops with much larger inter-element spacing, which was expected since the loop array with larger inter-element spacing was designed to act like a single element array. The stronger edge effect is especially shown by variations in the amplitude and phase values among the columns of elements near the edge of the closely-spaced array as shown by results derived from a line scan analysis. It should be noted that although it is advantageous that the square loop arrays with greater inter-element spacing had resonances that were less perturbed towards the edge of the array compared to the closely-spaced loops, there was much less absorptivity due to a lower fill factor and it is expected that these structures may show significant diffraction as well based on previous reports [7,10,22]. Based on previous work with truncated arrays, which suggested that loop elements would undergo a gradual blue shift of their peak resonance approaching the edge of large arrays, we expected that this same trend would occur here and be shown as a gradual decrease in near-field amplitude and gradual shift of the near-field phase [15]. However, the lack of this trend suggests that an additional near-field mode is being excited at the edge of the array.

Thus, to investigate the possibility of additional modes being excited at the edge of the closely-spaced array it became of interest to simulate the local spectral absorptivity among the individual loop elements near the edge of the array. Spatial absorptivity simulations have been useful in characterizing the resonant behavior of truncated arrays, so we applied this same method to characterize the spatial absorptivity at the edge of these closely-spaced square loop arrays [15]. Specifically, these simulations were performed by modeling a quasi-
infinite array, which was exited with an s-polarized, plane wave at 60° off-normal. The array size was determined to be quasi-infinite by observing that several columns in the middle of the array showed no discernable difference in the amplitude and phase of the near-field values. The spatial absorptivity was determined by integrating the volume loss density within the volumes representing the materials in each unit cell towards the edge of the array at different incident wavelengths. Then, the power absorbed by each unit cell at the edge and several unit cells away from the edge of the array was plotted versus wavelength. The resulting spatial absorptivity per unit cell showed two clear peaks in many of the spectra, which we attribute to two different resonances. Representative spectra of the power absorbed by the 5th through 9th columns of loops is shown in Fig. 7. One resonance is presumably due to the dipolar resonance of the elements, but the origin of the second resonance is unclear. In the previous far-field measurements of the local absorptivity we could not resolve the absorptivity among individual elements, but only locally among several elements, so this could explain the absence of this additional resonance in these measurements. In Fig. 8 the location of the resonant wavelength for each resonance was plotted as function of element number (where element “1” is the element at the edge of the array). It can be seen that both resonances become red-shifted (shifted to longer wavelengths) for elements further away from the edge of the array. It has been observed at lower frequencies that for finite arrays surface waves are often excited and become quite strong when the array is excited with incident radiation that is slightly off resonance [22]. Also, near the edge of a large array, edge waves typically can be excited, which decay as they travel away from the edge [22,38]. Since the arrays in this study are relatively large, this implies that this resonance is from edge waves and not from surface waves generated from small finite arrays. Confirming the existence of these edge waves is important since it alters the local spectral response of these structures at the edge of these quasi-infinite arrays compared to the response towards the center of the array. Also, even though these results suggest that the existence of these edge waves are highly dependent on inter-element spacing, this phenomenon should be applicable to many other quasi-infinite arrays where significant coupling is present.

Fig. 8. Plot of the location of the resonant wavelength for the two resonances observed in Fig. 7 vs element number. These results are derived from simulations of the spatial absorptivity of the closely-spaced array of loops on ZnS when illuminated at 60° off-normal. The red lines are present as a guide to the eye and are the result of a moving average applied to the points.
5. Conclusion

We investigated the effect of coupling among elements at the edge of arrays of square loops on ZnS in the near- and far-field. We expected the coupling to become diminished towards the edge of the closely-spaced loop arrays and to observe evidence consistent with a blue shift in the peak resonance. Indeed, we observed a blue shift of the peak resonance position by FT-IR where average responses over several elements was measured. However, interestingly, the simulated and experimental near-field results indicated that another resonance associated with the edge of the array is present, which we attribute to the excitation of an edge wave. Specifically, this is strongly suggested by both the simulated spatial absorptivity results and measured near-field amplitude and phase data.

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