Theoretical Study of Terahertz Near-Field Enhancement Assisted by Shape Resonance in Rectangular Hole Arrays in Metal Films

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(Received 19 November 2008)

We report a theoretical investigation on terahertz near-field enhancement in a rectangular hole array on a metal film driven by a shape resonance. The analytic model is constructed by boundary matching the Rayleigh wave expansion and the modal expansion of electromagnetic waves. Simulation results reveal that the enhancement factor depends on the inverse coverage, reaching more than 1000 in a sub-micron wide rectangular hole. We also show that the resonance frequency is predominantly determined by the length of the rectangles while variations in the width and the thickness cause minor shifts in the resonant frequency.

PACS numbers: 42.25.Fx, 78.66.Bz

Keywords: Terahertz, Near-field, Rectangular hole, Diffraction theory, Field enhancement

I. INTRODUCTION

Accumulation of the electromagnetic field into sub-wavelength structures such as holes [1–5], slits [6–8,21], particles [9] and wires [10] has been of great interest in a wide range of spectra from terahertz (THz) to visible frequencies. The major issue in this phenomenon is how to localize the field into the subwavelength region without losing significant energy. The conventional optical technique has a definite limit defined by the diffraction limit or Abbe limit [11]. Near-field scanning optical microscopy (NSOM) has made it possible to localize the field into the subwavelength region while sacrificing many parts of the energy subject to Bethe's criteria [12].

Investigation of transmission enhancement through a subwavelength aperture gives clear insight into this problem. Various resonance phenomena, such as surface plasmon polariton excitation [3,13], Fabry-Perot resonance [14], antenna resonance [10,15,16] and shape resonance [17,18], have been suggested as an efficient tool for accumulating energy through a subwavelength structure. In particular, it has been proven that the shape resonance plays a crucial role in field accumulation accompanied by the perfect transmission of THz field through the sub-

wavelength rectangular holes [17,19]. The field enhancement factor in a rectangular hole arrays on a metallic film is inversely proportional to the coverage, which is defined by the fractional area of the region of the opening relative to the total film. In this case, the rectangular hole acts as an optical resonator, whose function is essentially the same as that of the antenna in the microwave and radio frequency region.

In this paper, we present a theoretical study on the near-field and the far-field electromagnetic (EM) field distribution both in the spectral and the spatial domain for periodic rectangular arrays. Our simulation results reveal that perfect transmission is possible even in sub-micron-wide rectangles and that the field enhancement factor truly depends on the coverage. We also demonstrate that the length of the rectangles dominantly determines the resonance frequency while changes in the width and the thickness lead to minor shifts of the resonance.

II. THEORETICAL MODEL

1. Rayleigh Wave Expansion and Waveguide Mode Expansion

Figure 1 shows the model structure that is applied to

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Fig. 1. Schematic diagram of the sample geometry. The transmission region, the aperture region and the reflection region are assigned as regions I, II and III, respectively.

our simulation, together with coordinate assignments. Rectangles whose length and width are l and w , respectively, are punctured on a perfect metal film with thickness h . They are periodically aligned so that reciprocal vector is given as $\alpha_x = 2\pi/d_x$ and $\beta_y = 2\pi/d_y$, respectively. The TM polarized (electric field is along x direction) EM wave is incident normally. The EM fields on both sides of the reflection and the transmission can be obtained by using the Rayleigh wave expansion. The boundary condition is applied on each interfaces between the reflection side (region I) and the hole region (region II) and between the transmission side (region III) and the region II. Basically, both the reflected and the transmitted waves can be described as summations of the Fourier components whose bases vectors are α_x and β_y . Hence, the EM wave in region I and region III can be expressed as follows, respectively:

$$(H_x^I, H_y^I, H_z^I) = \sqrt{\frac{\varepsilon_0}{\mu_0}} \sum_{mn} (G_{mn}^x, G_{mn}^y, G_{mn}^z) \times e^{i\chi_{mn}(z-\frac{h}{2})} \times e^{i(\phi_{mn}-\omega t)} + e^{ik(z-\frac{h}{2})}, \quad (1)$$

$$(H_x^{III}, H_y^{III}, H_z^{III}) = \sqrt{\frac{\varepsilon_0}{\mu_0}} \sum_{mn} (F_{mn}^x, F_{mn}^y, F_{mn}^z) \times e^{-i\chi_{mn}(z-\frac{h}{2})} \times e^{i(\phi_{mn}-\omega t)}. \quad (2)$$

We use the magnetic field, not the electric field, because it is more convenient when we apply the boundary conditions. G 's and F 's denote Fourier amplitudes for each diffraction order in regions I and III, respectively. ϕ_{mn} denotes a spatial phase component along the xy -plane and is defined as $\phi_{mn} = \alpha_m x + \beta_n y$. χ_{mn} denotes a wavevector of each component along the z direction and is defined as $\chi_{mn}^2 = k^2 - \alpha_m^2 - \beta_n^2$. ε_0 and μ_0 denote the vacuum permeability and the permittivity, respectively. On the other hand the EM waves in region II can be obtained by EM waveguide expansion. Therefore, the general expression inside the rectangular hole region is

as follows:

$$\begin{aligned} \vec{H} &= (H_x, H_y, H_z) \\ &= \sum_{ij} (H_{ij}^{ox}(x, y), H_{ij}^{oy}(x, y), H_{ij}^{oz}(x, y)) \\ &\quad \times e^{i(\mu_{ij}z - \omega t)}. \end{aligned} \quad (3)$$

Again, μ_{ij} is a wavevector along the z direction, which is defined as $\mu_{ij} = \sqrt{k^2 - (k_x^i)^2 - (k_y^j)^2}$, where $k_x^i = \pi i/w$ and $k_y^j = \pi j/l$. Since w and l are smaller than the incident wavelength, μ_{ij} is forced to be imaginary. Especially, k_x^i is much larger than the incident wavevector k , so the contribution from the $i \neq 0$ terms is negligibly small because $e^{-|\mu_{ij}|z}$ decays very rapidly. In the same manner, the contribution from the $j > 1$ terms can be neglected; hence, we only need to consider the TE₀₁ mode. With this consideration, the magnetic field in region II is described as follows:

$$\begin{aligned} H_x^{II} &= 0 \\ H_y^{II} &= -\frac{i\mu}{k} \sqrt{\frac{\varepsilon_0}{\mu_0}} \sin\left(\frac{\pi y}{l}\right) \\ &\quad \times \left(A \frac{\sin \mu z}{\sin(\frac{\mu h}{2})} + B \frac{\cos \mu z}{\cos(\frac{\mu h}{2})} \right), \\ H_z^{II} &= +\frac{i}{k} \frac{\pi}{b} \sqrt{\frac{\varepsilon_0}{\mu_0}} \cos\left(\frac{\pi y}{l}\right) \\ &\quad \times \left(-A \frac{\cos \mu z}{\sin(\frac{\mu h}{2})} + B \frac{\sin \mu z}{\cos(\frac{\mu h}{2})} \right) \end{aligned} \quad (4)$$

where A and B denote the waveguide mode amplitudes and $\mu = \mu_{01} = \sqrt{k^2 - (\pi/l)^2}$.

2. Boundary Matching of the EM Field

To solve Fourier amplitude vectors F, G, A and B , boundary conditions at the I-II and the II-III interfaces are applied as follows:

$$\begin{cases} \left. \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right|_{III} = \left. \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right|_{II} \\ \left. -\frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} \right|_{III} = \left. \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} \right|_{II} \end{cases} \text{ at } z = -h/2, \quad (5)$$

$$H_y^{III} = H_y^{II} \text{ at } 0 \leq x \leq w, \ 0 \leq y \leq l, \ z = -h/2, \quad (6)$$

$$\begin{cases} \left. \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right|_I = \left. \frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} \right|_{II} \\ \left. -\frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} \right|_I = \left. \frac{\partial H_z}{\partial x} - \frac{\partial H_x}{\partial z} \right|_{II} \end{cases} \quad \text{at } z = h/2, \quad (7)$$

$$H_y^I = H_y^{II} \text{ at } 0 \leq x \leq w, \ 0 \leq y \leq l, \ z = -h/2, \quad (8)$$

Besides the boundary conditions, $\nabla \cdot \vec{H} = 0$ is also needed. From this relation, the z components of the

magnetic field can be substituted with y and z components as follows:

$$F_{mn}^z = \frac{1}{\chi_{mn}} (\alpha_m F_{mn}^x + \beta_n F_{mn}^y), \quad (9)$$

$$G_{mn}^z = -\frac{1}{\chi_{mn}} (\alpha_m G_{mn}^x + \beta_n G_{mn}^y). \quad (10)$$

Combining Eqs. (5) and (9) with Eqs. (7) and (10), respectively, gives the following relations:

$$\sum_{mn} \left(i \frac{\chi_{mn} k^2}{\chi_{mn}^2 + \alpha_m^2} \right) F_{mn}^y e^{i\phi_{mn}} = \begin{cases} ik \sin\left(\frac{\pi y}{b}\right) \left(A \cot \frac{\mu h}{2} + B \tan \frac{\mu h}{2} \right) & 0 \leq x \leq w, \ 0 \leq y \leq l \\ 0 & \text{otherwise} \end{cases}, \quad (11)$$

$$\sum_{mn} \left(i \frac{\chi_{mn} k^2}{\chi_{mn}^2 + \alpha_m^2} \right) G_{mn}^y e^{i\phi_{mn}} - ik \delta_{m0} \delta_{n0} = \begin{cases} -ik \sin\left(\frac{\pi y}{b}\right) \left(A \cot \frac{\mu h}{2} - B \tan \frac{\mu h}{2} \right) & 0 \leq x \leq w, \ 0 \leq y \leq l \\ 0 & \text{otherwise} \end{cases}. \quad (12)$$

Also from Eqs. (6) and (8), the following relations can be identified:

$$\sum_{mn} F_{mn}^y \times e^{i\phi_{mn}} = -\frac{i\mu}{k} \sin\left(\frac{\pi y}{b}\right) (-A + B), \quad (13)$$

$$\begin{aligned} \sum_{mn} (G_{mn}^y \times e^{i\phi_{mn}} + \delta_{m0} \delta_{n0}) \\ = -\frac{i\mu}{k} \sin\left(\frac{\pi y}{b}\right) (A + B). \end{aligned} \quad (14)$$

Integrating Eqs. (13) and (14) over the rectangular area gives the following:

$$\sum_{mn} F_{mn}^y J_{mn} = \frac{i\mu}{k\pi} (A - B), \quad (15)$$

$$\sum_{mn} G_{mn}^y J_{mn} + \frac{1}{2} = -\frac{i\mu}{k\pi} (A + B). \quad (16)$$

Similarly, the integration of Eqs. (11) and (12) over one unit cell gives the following relations:

$$\frac{\chi_{mn} k^2}{\chi_{mn}^2 + \alpha_m^2} F_{mn}^y = k K_{mn} \left(A \cot \frac{\mu h}{2} + B \tan \frac{\mu h}{2} \right), \quad (17)$$

$$\begin{aligned} i \frac{\chi_{mn} k^2}{\chi_{mn}^2 + \alpha_m^2} G_{mn}^y - ik \delta_{m0} \delta_{n0} \\ = -ik K_{mn} \left(A \cot \frac{\mu h}{2} - B \tan \frac{\mu h}{2} \right), \end{aligned} \quad (18)$$

where

$$J_{mn} = \frac{1}{2ab} \int_0^b \int_0^a e^{i\phi_{mn}} dx dy, \quad (19)$$

$$K_{mn} = \frac{1}{d_x d_y} \int_0^b \int_0^a \sin \frac{\pi y}{b} e^{-i\phi_{mn}} dx dy. \quad (20)$$

It is noticeable that J_{mn} is the Fourier-decomposed amplitude of the rectangle geometry and K_{mn} denotes the Fourier-decomposed overlap integral of the EM waveguide mode inside the rectangle. Eqs. (17) to (20) are coupled matrix equations for the 4 unknown vectors F, G, A and B . Solving these equations gives

$$A = \frac{1}{2 \left(W_x \cot \frac{\mu h}{2} - \frac{i\mu}{k\pi} \right)}, \quad (21)$$

$$B = \frac{-1}{2 \left(W_x \tan \frac{\mu h}{2} + \frac{i\mu}{k\pi} \right)}, \quad (22)$$

$$\begin{aligned} F_{mn}^y = \frac{\chi_{mn}^2 + \alpha_m^2}{\chi_{mn} k} \\ \times K_{mn} \frac{\frac{i\mu}{k\pi}}{\left(W_x^2 + \left(\frac{\mu}{k\pi} \right)^2 \right) \sin \mu h + 2 \frac{i\mu}{k\pi} W_x \cos \mu h}, \end{aligned} \quad (23)$$

$$G_{mn} = 1 - \frac{\chi_{mn}^2 + \alpha_m^2}{\chi_{mn}k} \times K_{mn} \frac{W_x + \frac{i\mu}{k\pi} \cot \mu h}{\left(W_x^2 + \left(\frac{\mu}{k\pi}\right)^2\right) + 2W_x \frac{i\mu}{k\pi} \cot \mu h}, \quad (24)$$

where W_x is given by

$$W_x = \sum_{mn} \frac{\chi_{mn}^2 + \alpha_m^2}{\chi_{mn}k} K_{mn} J_{mn}. \quad (25)$$

From these results, the electric and the magnetic field components are reconstructed in each region. For example, the electric field in the transmission region is given as follows:

$$E_x = \sqrt{\frac{\varepsilon_0}{\mu_0}} \sum_{mn} \left(K_{mn} \frac{W_x + \frac{i\mu}{k\pi} \cot \mu h}{\left(W_x^2 + \left(\frac{\mu}{k\pi}\right)^2\right) + 2W_x \frac{i\mu}{k\pi} \cot \mu h} \right) e^{i\chi_{mn}(z - \frac{h}{2})} \times e^{i(\phi_{mn} - \omega t)}, \quad (26)$$

$$E_y = 0, \quad (27)$$

$$E_z = \sqrt{\frac{\varepsilon_0}{\mu_0}} \sum_{mn} \left(\frac{\alpha_m}{\chi_{mn}} K_{mn} \frac{\frac{i\mu}{k\pi}}{\left(W_x^2 + \left(\frac{\mu}{k\pi}\right)^2\right) \sin \mu h + 2W_x \frac{i\mu}{k\pi} \cot \mu h} \right) e^{i\chi_{mn}(z - \frac{h}{2})} \times e^{i(\phi_{mn} - \omega t)}. \quad (28)$$

III. RESULT

1. Period Dependence

One of our primary concerns is the effective scattering cross-section for the rectangle resonator. To check this, we calculated zeroth order transmission spectra for rectangular arrays with different unit cell sizes. Figure 2 shows five different zeroth-order transmission spectra as the unit cell size changes from $1.5l$ to $3.5l$. The length and the width of the rectangle are fixed at $200 \mu\text{m}$ and $10 \mu\text{m}$, respectively. The transmission peaks remain at 1 for unit cell sizes smaller than $(2l)^2$. However, the transmission decreases rapidly from $(2.4l)^2$ until reaches ~ 0.2 for $(3l)^2$. This means that the rectangle resonator can accumulate the EM field region without losing any EM energy, as long as the unit cell is smaller than $\sim (2.4l)^2$.

2. Length, Width and Thickness Dependence

As shown in Figure 2, the spectral peak is found around the half-wavelength resonance. To demonstrate the change of the peak position explicitly, we vary the lengths of the rectangles from $200 \mu\text{m}$ to $350 \mu\text{m}$ while fixing the other values such that the period is $400 \mu\text{m}$, the thickness is $17 \mu\text{m}$ and the width is $10 \mu\text{m}$. Figure 3 shows the calculated zeroth order transmission for

different l values of $200, 250, 300$ and $350 \mu\text{m}$. As expected, strong red-shifts of the transmission peaks are observed as l increases while the perfect transmission is maintained. The peak position increases linearly as a function of l , as shown in the inset of Figure 3. The magnitude of the shift is about $130 \mu\text{m}$ when l increases by an amount of $50 \mu\text{m}$. This indicates that the shape resonance is basically the half-wavelength antenna resonance although a minor resonance shift is also expected, which is governed by other geometrical factors. It is also noticeable that the transmission dips found at 0.75 THz and 1.5 THz (which correspond to $200 \mu\text{m}$ and $400 \mu\text{m}$ in wavelength, respectively) do not change with length. This reflects that the interference driven by periodicity contributes negatively to the transmittance, which is referred to as Rayleigh minima [13] or Wood's Anomaly [20], in the optical region with a one-dimensional periodic structure.

To find the detailed dependencies on the width and the thickness, we performed a series of calculations for a fixed period of $400 \mu\text{m}$ and a length of $200 \mu\text{m}$. Figure 4 (a) shows the zeroth-order transmittance when the width is varied from $10 \mu\text{m}$ to $0.5 \mu\text{m}$ for fixed thickness of $17 \mu\text{m}$. As in the case of the length dependence, we can clearly observe resonance shifts for different widths of the rectangles. However, as shown in the inset of Figure 4(a), the resonance shift does not linearly depend on the width. With the assumption of a simple power law equation of $\lambda_{res} \sim w^\alpha$, we found that α can be estimated

Fig. 2. Zeroth-order transmittance for different unit cell sizes from $(1.5l)^2$ to $(3.5l)^2$.

Fig. 3. Zeroth-order transmittance for different lengths of the rectangles from $200 \mu\text{m}$ to $350 \mu\text{m}$. (Inset) Plot of the peak position as a function of the length l .

as ~ 0.5 .

Finally in Figure 4 (b), we show the zeroth-order transmittance when the thickness is varied from $0.5 \mu\text{m}$ to $35 \mu\text{m}$ for a fixed width of $5 \mu\text{m}$. Also shown in the inset is a plot of the peak positions as a function of the film thick-

Fig. 4. (a) Zeroth-order transmittance for six different rectangular widths from $0.5 \mu\text{m}$ to $10 \mu\text{m}$. (Inset) Peak position as a function of the width. (b) Zeroth-order transmittance for seven different thicknesses of the film from $0.5 \mu\text{m}$ to $35 \mu\text{m}$. (Inset) Peak position as a function of the thickness.

ness. The spectral peaks show clear blue-shifts whose magnitudes are inversely proportional to the thickness. Combining these considerations, we found that the relation between the resonance peak position and the geometrical factors can be summarized into

$$\lambda_{res} \sim 2l(a + k \frac{lw^{1/2}}{h}), \quad (29)$$

where k is a positive coefficient.

3. Near-field Enhancement and Coverage

As mentioned already, perfect transmission through the narrow rectangular holes strongly suggests that the electromagnetic field is accumulated in the near-field region. To confirm this, we calculated the near-field amplitude of the E_x component at $z = h/2$, $x = w/2$ and $y = l/2$ from Eq. (26). The length, thickness and period of the rectangle is fixed at $l = 200 \mu\text{m}$, $h = 5 \mu\text{m}$ and

Fig. 5. (a) E_x field amplitudes for six different widths of the samples in the near-field for $x = w/2$, $y = l/2$ and $z = 0$. (b) Enhancement factor and inverse coverage β^{-1} as functions of the width variation. (c) Cross-sectional plot of the electric-field magnitude along the xz -plane ($h = 17 \mu\text{m}$).

$d_x = d_y = 400 \mu\text{m}$; only the width is varied from $0.5 \mu\text{m}$ to $10 \mu\text{m}$ to change the coverage β . As shown in Figure 5(a), the near-field amplitude is dramatically enhanced, reaching ~ 1200 in the case of $w = 0.5 \mu\text{m}$, which corresponds to an inverse coverage of 1600. Note that this calculation is for the amplitude; hence, the intensity enhancement, which is the square of the amplitude, would be as large as $\sim 10^6$. The enhancement factor, as well as the inverse coverage β^{-1} , is plotted in Figure 5(b) as a function of the rectangular width. As shown in the figure, the enhancement factor matches well with the inverse coverage, except for the case of $w = 0.5 \mu\text{m}$, where the damping effect starts to show up.

The cross-sectional plot along the xz -plane reveals that the field enhancement is truly due to the field ac-

cumulation inside the rectangular aperture. Figure 5(c) shows a plot the electric field amplitude as functions of x and z for a sample with $w = 5 \mu\text{m}$, $h = 17 \mu\text{m}$, $l = 200 \mu\text{m}$ and $d_x = d_y = 400 \mu\text{m}$. It is clear that the electric field on the reflection side of film is accumulated, which results in a dramatically enhanced field inside the rectangular aperture. Subsequently, the transmitted field re-radiates, following a dipole-like radiation pattern. We should like to emphasize that the field enhancement is strongly localized only near and inside the holes, which should stimulate a future applications of subwavelength imaging and novel THz nonlinear spectroscopies.

IV. CONCLUSIONS

In conclusion, we have demonstrated theoretically the electromagnetic field distribution both in the near-field and the far-field regions of a rectangular hole array. Through the calculation of the far-field spectrum, the resonance frequency shifts due to the length, width and thickness variations were explicitly demonstrated and were expressed in the a form of a simple formula. On the other hand, the near-field image confirmed the field accumulation near and inside the apertures. The field enhancement factor followed an inverse coverage β^{-1} .

ACKNOWLEDGMENTS

This work was supported by a Korea Research Foundation grants funded by the Korean Government (KRF-2007-412-J04002, KRF-2008-331-C00103). The work is also supported by Korea Science and Engineering Foundation grants (R11-2008-095-01000-0, R01-2008-000-20702-0).

REFERENCES

- [1] T. W. Ebbesen *et al.*, Nature **391**, 667 (1998).
- [2] S. C. Hohng *et al.*, J. Korean Phys. Soc. **46**, (2005).
- [3] W. L. Barnes *et al.*, Phys. Rev. Lett. **92**, 107401 (2004).
- [4] F. J. Garcia-Vidal *et al.*, Phys. Rev. B **74**, 153411 (2006).
- [5] A. Bitzer and M. Walther, Appl. Phys. Lett. **92**, 231101 (2008).
- [6] D. J. Park *et al.*, Phys. Rev. B **77**, 115451 (2008).
- [7] J. W. Lee *et al.*, J. Korean Phys. Soc. **48**, 103 (2006).
- [8] S. Choi *et al.*, J. Korean Phys. Soc. **53**, 713 (2008).
- [9] S. K. Eah, W. Jhe and Y. Arakawa, Appl. Phys. Lett. **80**, 2779 (2002).
- [10] J. Aizpurua *et al.*, Phys. Rev. B **71**, 235420 (2005).
- [11] E. Abbe, Archiv f. Mikroslop. Anat. **9**, 413 (1873).
- [12] H. A. Bethe, Phys. Rev. **66**, 163 (1944).
- [13] Q. Cao and P. Lalanne, Phys. Rev. Lett. **88**, 574031 (2002).

- [14] J. E. Kihm *et al.*, Phys. Rev. B **75**, 035414 (2007).
- [15] P. Muhlschlegel *et al.*, Science **308**, 1607 (2005).
- [16] L. Novotny, Phys. Rev. Lett. **98**, 266802 (2007).
- [17] J. W. Lee *et al.*, Phys. Rev. Lett. **99**, 137401 (2007).
- [18] J. W. Lee *et al.*, Opt. Exp. **14**, 12637 (2006).
- [19] F. J. Garcia-Vidal *et al.*, Phys. Rev. Lett. **95**, 103901 (2005).
- [20] R. W. Wood, Phys. Rev. **48**, 928 (1935).
- [21] J. H. Kang *et al.*, J. Korean Phys. Soc. **49**, 881 (2006).