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### Optimal arrangement of meta-atoms composing metamaterials

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#### **ABSTRACT**

In order to better understand how to improve the performance of a superlens, structural and geometrical arrangements of meta-atoms are investigated. Each meta-atom (i.e. the unit element composing a metamaterial) in our study is an asymmetric 3D "S"-shaped resonator. This structure radiates an enhanced scattered field at several possible resonant frequencies, some of which are out of phase with the incident wave. We retrieve the effective parameters of different metamaterials and discuss the role of meta-atom symmetries and dimensions in affecting the effective refractive index of a metamaterial slab. Relative locations and orientations of individual meta-atoms are investigated to provide desired properties with low loss despite the inevitable finite size of each meta-atom. The results presented provide insights for designing superlenses, resonant antennas, and other potential applications.

**Keywords:** Metamaterials, superresolution, field enhancement, resonant scattering, superlens

#### 1. INTRODUCTION

#### 1.1 Negative index metamaterials and superresolution imaging

Our motivation is to understand how to assemble a practical metamaterial with a refractive index close to -1 which can be used for high resolution (sub-wavelength scale) imaging. We do not expect to be able to make the "perfect" lens with these properties but, by adjusting the components of our metamaterial, to maximize the transfer of evanescent waves from the 3D scattering object to the image domain. Transfer of evanescent waves, or equivalently, high spatial frequencies with  $k > k_0$ , will lead to a field pattern in the image domains exhibiting superoscillations. It will remain an important and as yet unanswered question how to relate this field pattern to the intrinsic material properties of the object to be imaged: this represents an inverse scattering problem to be addressed in a later publication. The successful transfer of some bandwidth of evanescent waves will improve resolution and thereby increase the effective number of degrees of freedom of the imaging system. Some evanescent waves might be coupled into propagating waves which of course is the express purpose of a hyperlens. The latter is highly desirable but the inverse scattering problem remains and there is the potential for the cross-contamination of converted evanescent waves into k-vectors associated with propagating scattered field components from the object. We view the transfer of evanescent waves as inherently a multiple scattering and element-to-element coupling phenomenon. Consequently, the shape and proximity of the elements or meta-atoms used in the design of our bulk metamaterial play a critical role in high spatial frequency transfer. If the ideal metamaterial for perfect imaging has an index of -1, then it is likely that the optimized but practical metamaterial we seek will also exhibit a negative index. This property is well known to be associated with group and phase velocities having opposite directions. Normally, we attribute a positive index to naturally occurring materials based on its approximate description in terms of a large number of dipole radiators, each representing an atom in that material. The sum of the fields from a sheet of diploes can be calculated and it is found to lead to an overall phase retardation with respect to the incident or

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driving field, and this delay is considered synonymous with a positive refractive index. By analogy with this, one might expect that a combination of meta-atom location and non-dipole-like radiation patterns could provide an overall phase advance, characteristic of a negative refractive index. The 3D scattering or radiation (beam) pattern from each meta-atom determines the phase, amplitude and direction of the wave transferred to its neighbors in the metamaterial [1]. Providing these meta-atoms in close proximity to each other, there is an opportunity for evanescent waves to be coupled and transferred through the structure. One usually assumes phase advance or retardation shifts accumulate gradually during the wave's propagation through a material, to shape emerging wavefronts and beams. Meta-atoms, however, can introduce abrupt phase changes over scales shorter than the wavelength [1]. Even a two-dimensional array of resonant meta-atoms with spatially varying phase response and subwavelength separations can impose extreme phase shifts (even discontinuities) on propagating electromagnetic waves, leading to anomalous reflection and (negative) refraction phenomena, which have been observed. Our question is how we exploit this to faithfully transfer the widest bandwidth of evanescent waves in a practical metamaterial.

#### 1.2 Methods to identify negative refraction and/or negative refractive index

There are several methods to identify negative refractive properties in a metamaterial. Simple examples include i) negative refraction phenomenon observed in a prism made of a negative refractive metamaterial [2]; ii) observation of a backward wave and phase advance in a negative refractive index metamaterial [3, 4]; iii) the transmission spectrum of evanescent incident waves shows pass bands (i.e. if there is no negative refraction, a structure illuminated with evanescent waves will show no transferred wave) [5]. Alternatively, one may also calculate the refractive index of a metamaterial using, for example, the S-parameter retrieval method [6, 7], to determine if the metamaterial shows negative refractive index.

The S-parameter retrieval method is widely used to obtain effective parameters of a metamaterial, including refractive index (n), permittivity  $(\varepsilon)$ , and permeability  $(\mu)$ . We note that this approach has been scrutinized in some detail when applied to metamaterials, specifically because of the inherent periodicity of most metamaterials (see [7]) and great care must be taken in interpreting the calculated estimates for refractive index. In the retrieval method, S-parameters  $(S_{11}$  and  $S_{21}$  for example) are obtained experimentally and/or numerically. The impedance (Z) and n are then obtained by the following equations [6].

$$Z = \pm \sqrt{\frac{\left(1 + S_{11}\right)^2 - S_{21}^2}{\left(1 - S_{11}\right)^2 - S_{21}^2}} \tag{1}$$

$$e^{ink_0d} = \frac{S_{21}}{1 - S_{11} \frac{Z - 1}{Z + 1}} \tag{2a}$$

$$n = \frac{1}{k_0 d} \left\{ \left[ \left[ \ln \left( e^{ink_0 d} \right) \right]^n + 2\pi m \right] - i \left[ \ln \left( e^{ink_0 d} \right)^n \right] \right\}$$
 (2b)

where (') and (") denote the real part and imaginary part operators respectively, d is the thickness of the material in the propagation direction, and m is an integer that defines the branch of the complex logarithmic function. For a passive medium, the conditions that  $Z' \ge 0$  and  $n'' \ge 0$  (or equivalently,  $|e^{ink_0d}| \le 1$  [6]) must be fulfilled. The branch index m is zero at low frequencies, and the value of m for higher frequencies is determined by the mathematical continuity of the parameters, as described in [6].

#### 2. DOUBLE-LAYERED S-SHAPED STRUCTURE

It has been reported that S-shaped resonators (also called *meander line structure* [8-10]) can support negative refractive index properties and thus be used to compose a metamaterial superlens [8, 9]. In this study, two different double-layered "S"-like structures are investigated (Fig. 1). The structures under study compose of S-shape resonators (copper) printed on the opposite sides of a dielectric substrate (FR4, *E*=3.9). One contains two identical S-shape resonators (the *parallel* case) and the other one consists of mirrored S-shape resonators (the *mirrored* case). The mirrored case is very similar to the S-shaped split ring resonator (SRR) proposed by Chen et al. [8]. Here the dielectric constant of the materials used is assumed constant as a function of frequency for simplicity. Both structures are assumed continuously connected in the y-direction and the dimensions of the structures are chosen so that the resonant frequencies are in the range of 7 GHz to 12 GHz (Fig. 1(c)). The ratio of vacuum wavelength to unit cell size in the propagation direction is between 3.9 (at 12 GHz) and 6.7 (at 7 GHz). As a result of the structure's strong dispersion near resonant frequencies, it is not simple to specify how well such a meta-atom assembled into a metamaterial will behave as an anisotropic but continuous effective medium over the frequencies in this range. However, our primary goal is to investigate the transfer of evanescent waves since successful transfer, even if associated with distortions, need not preclude the successful computation of a superresolved image from the measured fields. A commercial software package, COMSOL (v.4.2), based on finite element method, is used to obtain S-parameters.

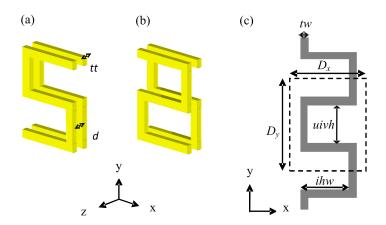


Figure 1. Basic double-layered S structures under study. Meta-element of (a) the parallel case (b) the mirrored case, (c) dimensions of the structures, where uivh=3.2 mm, ihw=3.84 mm, tw=0.64 mm, tt=38  $\mu$ m, and d=1.6 mm. This structure is made of copper and is printed on the opposite sides of a dielectric substrate (FR4,  $\varepsilon=3.9$ ) with the unit cell size  $D_y=7.68$  mm and  $D_x=6.4$  mm (indicated by the dashed rectangle in (c)). Both structures are assumed continuously connected in the y-direction.

#### 2.1 The parallel case

We started our investigation with the parallel design (Fig. 1(a)), assuming plane waves are normally incident on the y-z plane and propagating along the +x-direction with *E*-field polarized in y-direction. Periodic boundary conditions are applied on the domain boundaries parallel to the x-y plane and x-z plane so that the structure is assumed to be repeated infinitely in z-direction and y-direction respectively. The retrieved effective refractive index of one row, two rows, and three rows of the parallel S in the x-direction are displayed in Fig. 2, as a function of frequency. As seen in the figure, the retrieved refractive index of different rows of the parallel S are very similar, suggesting that a thin row of such parallel S can represent an effectively homogeneous metamaterial slab without considering the coupling between the neighboring rows. The loss is close to zero in the range of 9.1 GHz to 9.7 GHz, where the corresponding n' gradually changes from 0 to 1.8. This is an intriguing and important observation suggesting that for a chosen fixed frequency, the geometry of this parallel S structure could be altered in order to define any index over this range while maintaining low loss. However, for the given geometrical placement and material properties used, we have not found a condition for this parallel design to support a negative refractive index.

It was reported that negative refractive index can be achieved by breaking the geometrical symmetry (e.g. symmetry between the two stacked layers) and/or structural symmetry (i.e. the symmetry of the meta-atom structure) [13, 14]. We have also broken the structural symmetry of the S metamaterial by considering two rows in the propagation direction with one row shifted by  $0.5*D_y$  and 3\*tw, the retrieved results are very similar to the ones obtained in Fig. 2 and do not support a negative refractive index.

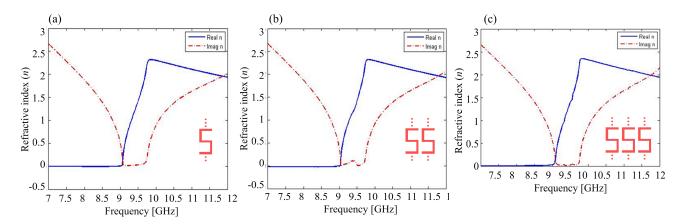


Figure 2. Effective refractive index of different rows of the parallel S structures in the x-direction. (a) One row, (b) two rows, and (c) three rows.

#### 2.2 The mirrored case

Similarly, we obtained the effective refractive index of the mirrored structure (with the same dimensions as the parallel case, indicated in Fig. 1(c)) as shown in Fig. 3(a). This structure was first studied in detail in [4]. The retrieved refractive indexes of one to three rows of the mirrored S in the propagation direction also match well, indicating that the properties of a single sheet dominate the resulting bulk metamaterial's properties. This structure supports a low loss negative refractive index from 7.8 GHz to 11 GHz, and n is approximately equal to -1 around 9.09 GHz. The low-loss frequency range in this case is wider compared to that for the parallel case.

To break structural symmetry of this S metamaterial, we considered the two rows in x case, with one row shifted by  $0.5*D_y$  and 2\*tw (Fig.3 (b) and (c)), the retrieved results are very similar to those obtained without breaking structural symmetry. This result is encouraging, suggesting some fabrication tolerance would be allowed for such a metamaterial, important if assembling it from layers and for eventual optical applications. Compared to the parallel cases, where a *step-like* curve is introduced in the retrieved refractive index spectrum when one row is shifted by  $0.5*D_y$ , the mirrored case does not have this trend.

Coupling between neighboring layers was also investigated. Fig. 4 shows the retrieved refractive index for different periodic spacings in the z-direction, assuming there is only one row in the forward propagation direction (+x). When the period in the z-direction increases (i.e. coupling becomes weaker), the low-loss frequency range of negative refractive index becomes smaller, and the frequency where n = -1 occurs also increases with  $D_z$ . The complex nature of the scattering pattern from a single meta-atom shows considerably asymmetry of the field in x and z but symmetry with the symmetry of the structure in y.

Fig. 5 shows how the refractive index of the mirrored case also changes with different trace width, another degree of freedom at our disposal for controlling the scattering and coupling between meta-atoms. When the trace width of the mirrored case is reduced from 640  $\mu$ m to 80  $\mu$ m, in general the frequency range of low-loss negative refractive index becomes smaller. The frequency at which n = -1 occurs, increases with reducing trace width, consistent with a reduction in both the capacitance and the inductance of the meta-atom. The curve shown in the tw=160  $\mu$ m case is a typical example demonstrating the effects due to structure periodicity; similar curves are reported in [10]. We normally expect a resonance-related negative index to be on the high frequency side of the resonant frequency. For the larger trace widths shown, the index behavior is indeed at a higher frequency than the resonant frequencies which are not shown (< 7GHz).

The figure for  $tw = 80 \mu m$  which has the highest resonant frequency, looks like a classical resonance phenomenon over our frequency range. In this case, there is no negative refractive index present but a sharp change of refractive index from 0 to 2.2 then back to 0 from 8.8 GHz to 9.3 GHz.

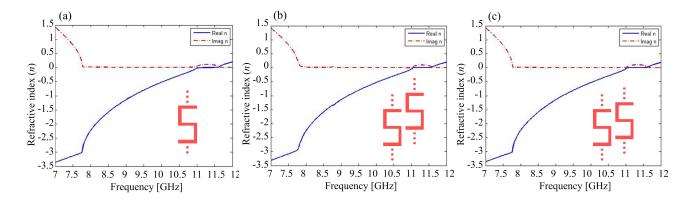


Figure 3. Effective refractive index of different rows of the mirrored S structures in the x-direction. (a) One row, (b) two rows, and (c) three rows. (d) Two rows with one row shifted by  $D_y/2=3.84$  mm (e) two with one row shifted by 2\*tw=1.28 mm

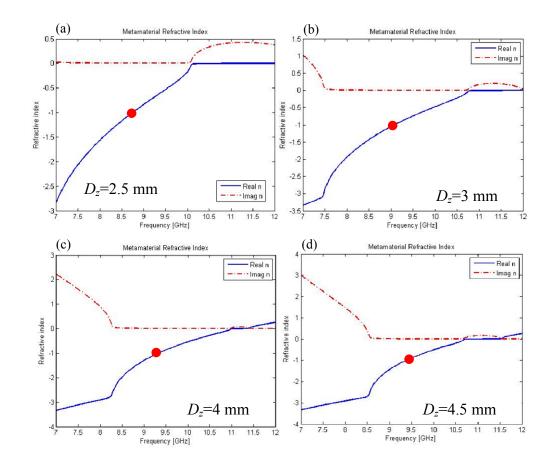


Figure 4. Effective refractive index of the mirrored S structures with different values of the period in the z-direction  $(D_z)$ . Red dot indicates where n=-1 occurs

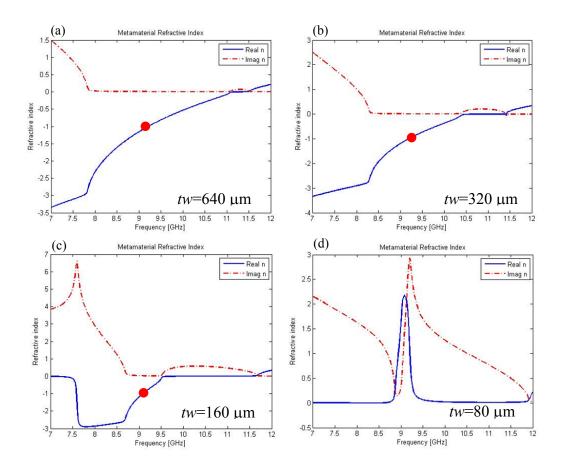


Figure 5. Effective refractive index of the mirrored S structures with different values of the trace width (tw), where uivh=3.2 mm and ihw=3.84 mm are assumed constant. Other design parameters also remain the same. Red dot indicates where n=-1 occurs.

#### **CONCLUSIONS**

We have described as systematic study into the design of a bulk metamaterial to be used for superresolved imaging. The meta-atoms employed are of a well-known type, parallel or mirrored S structures, which others have demonstrated are capable of supporting a negative index. Our point in this paper is that in developing practical metamaterials comprised of such meta-atoms there are several degrees of freedom available to enable the improved transfer of evanescent waves from the object to image domains. Having set a desired wavelength range of operation and a size for the meta-atoms, we presented results showing how adjustments to the proximity of meta-atoms to each other and the metal trace width, can control the effective complex refractive index of a periodic bulk metamaterial. We focused on a frequency range over which losses could be controlled to be relatively low (of the order of + i 0.02) and the real part of the refractive index could be varied from  $-3 \le n \le 2.5$  with different designs. For high resolution imaging applications, we have most interest over the design parameter set for which  $n \sim -1$  and losses are low. We established that bulk metamaterial properties are largely dictated by a periodic sheet of meta-atoms just one layer thick in the propagation direction. In other words, at least for the cases studied, the bulk metamaterial properties were not strongly influenced by the number of additional layers in the x direction, nor did the alignment of these layers with respect to y and z greatly affect the overall complex refractive index for this frequency range. The choice of trace width did modify the low loss and negative index regime for the mirrored structure and that modification was explained in terms of the associated dependence of the resonant frequency on trace width. Numerical simulations confirm a backward wave with low loss at the predicted frequencies but

finite size effects and determining the functional dependence of the evanescent wave transfer function on the parameters we adjusted is an on-going exercise and will be reported in a future publication.

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