Analysis of 2D hyperbolic metamaterial dispersion by elementary excitation coupling

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ABSTRACT

Hyperbolic metamaterials are examined for many applications thanks to the large density of states and extreme confinement of light they provide. For classical hyperbolic metal/dielectric multilayer structures, it was demonstrated that the properties originate from a specific coupling of the surface plasmon polaritons between the metal/dielectric interfaces. We show a similar analysis for 2D hyperbolic arrays of square (or rectangular) silver nanorods in a TiO2 host. In this case the properties derive from a specific coupling of the plasmons carried by the corners of the nanorods. The dispersion can be seen as the coupling of single rods for a through-metal connection of the corners, as the coupling of structures made of four semi-infinite metallic blocks separated by dielectric for a through-dielectric connection, or as the coupling of two semi-infinite rods for a through-metal and through-dielectric situation. For arrays of small square nanorods the elementary structure that explains the dispersion of the array is the single rod, and for arrays of large square nanorods it is four metallic corners. The medium size square nanorod case is more complicated, because the elementary structure can be one of the three basic designs, depending on the frequency and symmetry of the modes. Finally, we show that for arrays of rectangular nanorods the dispersion is explained by coupling of the two coupled rod structure. This work opens the way for a better understanding of a wide class of metamaterials via their elementary excitations.

Keywords: metamaterials, plasmonics, 2D crystal

1. INTRODUCTION

Metamaterials and their special light control abilities that are impossible with natural materials arouse a large interest over the last decade.[1–4] Among these developments hyperbolic metamaterials provide attractive properties such as a very large density of states[5] and refractive index,[6,7] thanks to their extreme anisotropy.[8] These engineered materials are a particular case of anisotropic media, where components of the diagonalized permittivity tensor have opposite sign, leading to new light-matter interaction phenomena.[9]

Two well-known structures provide for hyperbolic properties: a periodic metal-dielectric multilayer structure (Fig. 1a)[10–12] and an array of cylindrical metallic nanorods in a dielectric host.[13,14] The origins of the hyperbolicity in the multilayer configuration were shown to come from the plasmonic nature of the structure, specifically from the coupling of short-range surface plasmon polaritons that propagate in each unit cell of the periodic structure.[15,16]

In a more general way, a method introduced by Rosenblatt and Orenstein allows to understand the dispersion of the same structure as a competition between the elementary excitations of the structure.[17] These elementary excitations are namely the 'gap' modes and 'slab' modes, depending through which layer the coupling between the surface plasmons at each metal/dielectric interface occurs (through the metal for the slab and through the dielectric for the gap).

In this paper we propose an extension of this method for 2D arrays of square or rectangular silver nanorods in a TiO_2 host (Fig. 1b). The complexity of the method is higher in this case due of the higher number of modes and the fact that the Brillouin zone (BZ) for the transverse Bloch components k_x and k_y is two-dimensional.

We explain the geometry, notation and technique of analysis in Sec. 2. We demonstrate the dependance on the nanorod size of the elementary excitations that describe the dispersion of the array in the other Sections.

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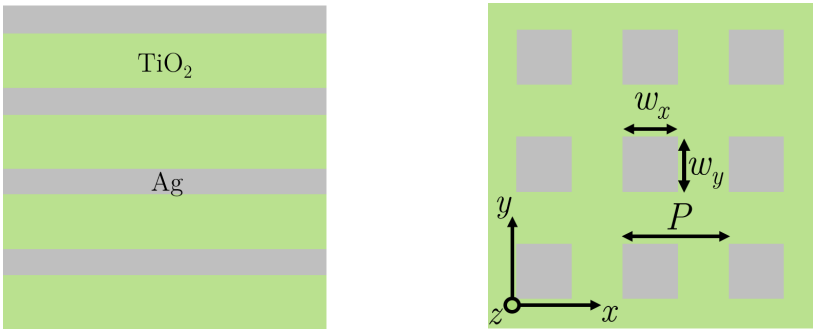


(a) (b)

Figure 1: (a) Metamaterial consisting of periodic subwavelength layers of silver (Ag) and TiO_2. (b) Metamaterial consisting of an array of square or rectangular silver nanorods in a TiO_2 host. w_x and w_y are the size of the nanorods in the x and y directions, P is the period of the array.

In particular, we show in Sec. 3 and 4 that the dispersion of arrays of small (compared to the period) and large square nanorods originates from the coupling of single rods and four-corner structures, respectively. The dependance on the frequency range mode symmetry for intermediate nanorod sizes is examined in Sec. 5. Finally, in Sec. 6 we break the symmetry between the x and y directions with rectangular nanorods with one dimension much larger than the other, finding that two coupled semi-infinite rods explains very well the dispersion of the periodic structure. We conclude in Sec. 7.

2. METHODS

2.1 Geometries

We study the dispersion of arrays of silver square and rectangular nanorods (with slightly rounded corner to avoid extreme hotspot) of various size in a dielectric TiO_2 host with periodicity P = 30 nm in both x and y directions. We take the refractive index of TiO_2 $n = 2.7$ and a lossless drude model for silver:

$$\varepsilon_{Ag}(\omega) = 1 - \frac{\omega_p^2}{\omega^2} \tag{1}$$

with $\omega_p = 1.26 \times 10^{16}$ Hz the plasma frequency.

Three different cases are examined for the square nanorod arrays: a first case with the width w of the rods being much smaller than the period ($w = 8$ nm, Fig. 2a), a second case with the width of the rods slightly smaller than the period ($w = 25$ nm, Fig. 2b), and a third case with an intermediate width ($w = 16.3$ nm, Fig. 2c).

(a) (b) (c) (d) (e)

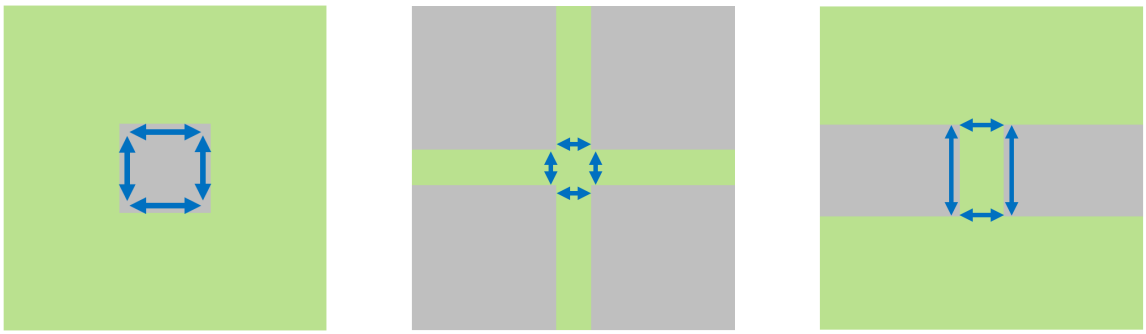
Figure 2: Single unit cell of the studied structures, the period in x and y direction is $P = 30$ nm: array of square nanorods with width (a) $w = 8$ nm, (b) $w = 25$ nm, (c) $w = 16.3$ nm. (d) Array of rectangular nanorods of width $w_x = 20$ nm and $w_y = 10$ nm. (e) Reciprocal lattice and first Brillouin zone (in light blue).

For the three cases the irreducible Brillouin zone is a triangle (Fig. 2e) delimited by three important points: the center of the BZ Γ where $k_x = k_y = 0$, the $X_1(X_2)$ point where k_x (k_y) is equal to $\frac{\pi}{P}$ and the M point where $k_x = k_y = \frac{\pi}{P}$.

The influence of breaking the symmetry between the x and y directions is also studied by examining another geometry of rectangular nanorod arrays with width in the x direction $w_x = 20$ nm much larger than the width in the y direction y direction $w_y = 10$ nm, Fig. 2d). Because of the asymmetry between x and y, the irreducible Brillouin zone is a square delimited by four points: Γ, X_1, X_2 and M.

Unlike the simple multilayer case, purely TM propagating modes do not exist here. All modes present the six components of the fields.[18] Thus it is very difficult to analytically study these lattices, and we employ a numerical solver COMSOL Multiphysics based on the finite element method. However, similarly to the method used by Rosenblatt and Orenstein for multilayers,[17] we look for elementary excitations that describe the array dispersions for each case.

The plasmonic mode guided by a metallic corner is the simplest excitation here (surface plasmon polaritons for the multilayer case). This corner plasmon can couple to their neigbouring corners in three different manners: through a dielectric layer, via a metallic edge of the rod or with a combination of the two (through dielectric in one direction and via metallic edge in the other). These three ways of coupling lead to three elementary structures: the single-rod structure (Fig. 3a), the four-corner structure (Fig. 3b) and the coupled-rod structure (Fig. 3c), respectively.



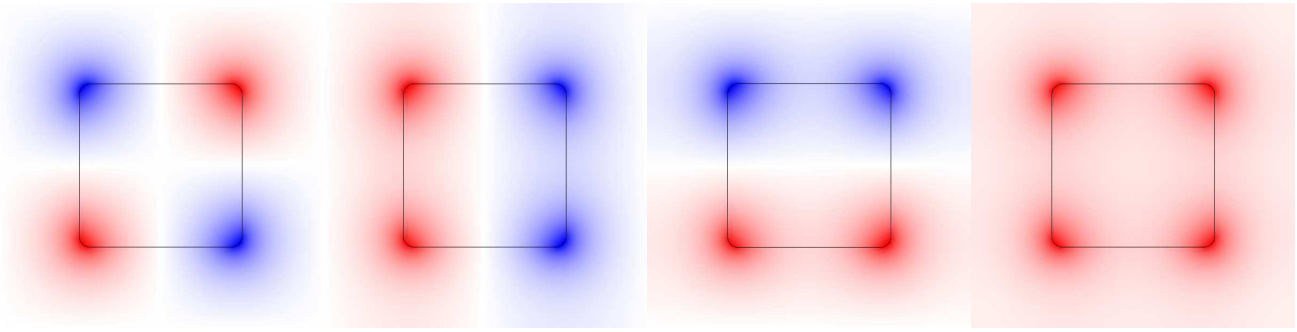
(a) (b) (c)

Figure 3: Elementary structures related to the arrays: (a) single rod in an infinite dielectric host. (b) Four metallic corners connected via dielectric medium. (c) Two coupled semi-infinite rods. Blue arrows indicate the principal ways of coupling between corners.

2.2 Notations

Four different symmetries for guided modes exist in our structures (Fig. 4). We use a simple notation to determine the modes based on their symmetry. A mode is described by two letters, the first letter represents the symmetry of E_z along a rod side in the x direction, and this letter can be "a" for asymmetric or "s" for symmetric field. The second letter represents the symmetry along a rod side in the y direction, with the same modalities. Note that we only focus on the lower order modes. Four possibilities are thus present : the aa mode (Fig. 4a), as mode (Fig. 4b), sa mode (Fig. 4c) and ss mode (Fig. 4d). We use the same nomenclature to distinguish the elementary structures.

Note that the sa and as modes for the arrays of square nanorods at the Γ and M points are degenerate. However, the sa and as modes are not degenerate at the X_1 (or X_2) point. The sa and as modes of the elementary structures are also degenerate for the single-rod and the four-corner structure but not degenerate for the coupled-rod case. Finally, the modes of the rectangular nanorod array and their elementary structure modes are not degenerate because of the symmetry breaking between x and y directions.



(a) *aa* (b) *as* (c) *sa* (d) *ss*

Figure 4: Component E_z of the electric field over a single unit cell for an array mode at the Γ point for $w = 16.3$ nm at $\lambda_0 = 700$ nm. (a) *aa* mode. (b) *as* mode. (c) *sa* mode. (d) *ss* mode.

2.3 Dispersion analysis method

A 2D extension of the method used in[17] is presented. The conclusion of the method is that the mean of the plasmonic band dispersion of a periodic structure corresponds with the dispersion of the elementary excitations of this structure. The mean of the plasmonic band for 2D arrays of square nanorods, where the irreducible Brillouin zone is a triangle, is calculated as

$$\omega_m(k_z) = \frac{\omega_a(\Gamma, k_z) + \omega_a(\mathrm{X}_1, k_z) + \omega_a(\mathrm{M}, k_z)}{3}. \tag{2}$$

For arrays of rectangular nanorods, where the irreducible Brillouin zone is a square we use

$$\omega_m(k_z) = \frac{\omega_a(\Gamma, k_z) + \omega_a(\mathrm{X}_1, k_z) + \omega_a(\mathrm{X}_2, k_z) + \omega_a(\mathrm{M}, k_z)}{4} \tag{3}$$

with $\omega_m(k_z)$ the mean of the plasmonic band for a given propagating constant k_z. $\omega_a(\Gamma, k_z)$, $\omega_p(\mathrm{X}_1, k_z)$, $\omega_a(\mathrm{X}_2, k_z)$ and $\omega_a(\mathrm{M}, k_z)$ are the frequencies of the propagating mode of the periodic array at the Γ, X_1, X_2 and M points, respectively.

We assume that a good correspondence between the mean of the plasmonic band and the dispersion of an elementary structure indicates that the array modes 'arise' from the modes of this elementary geometry, mathematically translated as

$$\omega_m(k_z) \approx \omega_e(k_z), \tag{4}$$

where $\omega_e(k_z)$ is the frequency of the elementary excitation for a given k_z.

To adequately apply equation 4, note that the symmetry of a given mode alongside a nanorod at the center of the Brillouin zone (Γ) is not necessarily the same at the X_1 and M points, so it requires caution when using equations 2 and 3 to calculate the mean of the plasmonic band.

3. SMALL NANORODS

We examine the dispersion for arrays of small (compared to the period) square nanorods with a width $w = 8$ nm. Using equation 2, we calculate the mean of the plasmonic band for each mode (so four means are calculated) and compare it to the adequate elementary excitation (Fig 5).

We see from Fig. 5 that the dispersion of the single-rod geometry corresponds very well with the calculated mean (the red dashed curve overlaps well with the blue solid curve) of the array. Therefore, according to our assumption (equation 4), the single-rod mode describes the array mode, and thus the corners are connected via metal-dielectric interfaces.

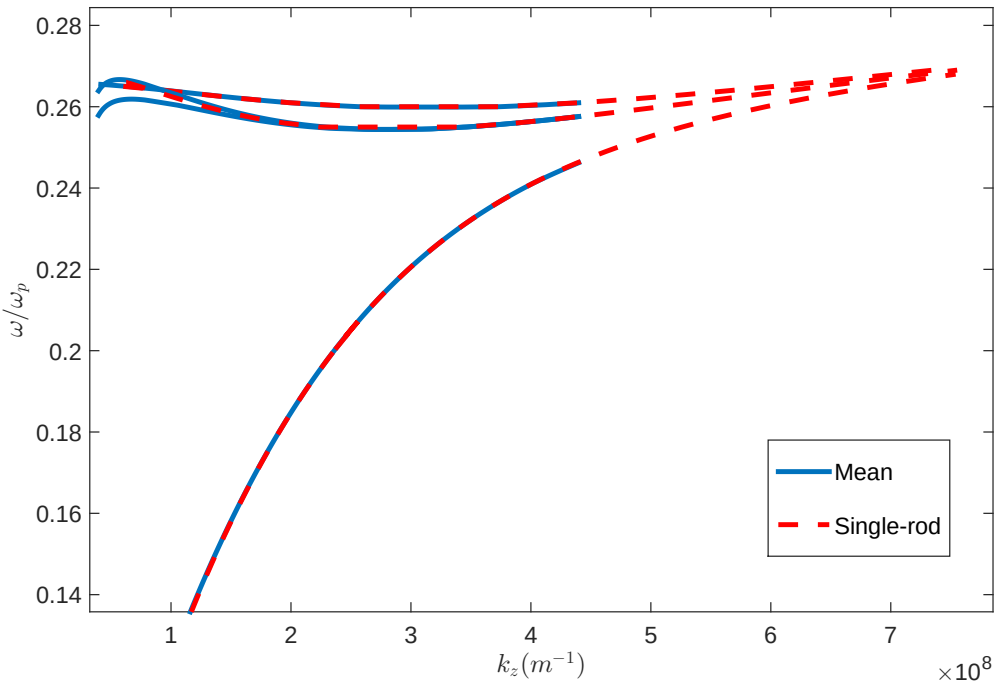


Figure 5: Comparison between the mean calculated with equation 2 and the single-rod excitation for the small nanorod array.

4. LARGE NANORODS

The same analysis is performed for large square nanorod arrays ($w = 25$ nm). Again, we use equation 2 to calculate the mean of the plasmonic band for each mode and compare it with the adequate elementary excitation (Fig. 6).

In this case, the calculated mean corresponds very well with the dispersion of the four-corner structure for each mode. This implies that the plasmonic mode of the large nanorod array originates from the four-corner structure, and thus the plasmonic corners mainly couple through the dielectric (Fig. 3b) and not via metal-dielectric interface as for the small nanorod case.

5. MEDIUM SIZE NANORODS

For medium size square nanorods we choose the width of the nanorods to be $w = 16.3$ nm. This particular size was chosen by examining the dispersion at the Γ point for varying widths. The aa mode dispersion is always above the ss mode for the small nanorod array (Fig. 7a). In the case of large nanorods however, the ss mode is above the aa mode curve (Fig. 7c). At the particular width $w = 16.3$ nm, the aa and ss curves intersect each other and the modes are very close (Fig. 7b), and we are thus in between the two regimes of the two previous Sections.

Again, using equation 2 we determine the mean for each mode (Fig. 8). Two different regimes are present here, delimited by the intersection frequency of the aa and sa/as modes curves, around $\omega = 0.246\ \omega_p$. Below $\omega = 0.246\ \omega_p$, we can see that the calculated mean corresponds very well with different elementary structures depending on the symmetry of the mode. In particular, the aa and as modes approach the coupled-rod structure dispersion, the sa mode approaches the dispersion of the single rod and the ss mode corresponds to the four-corner structure.

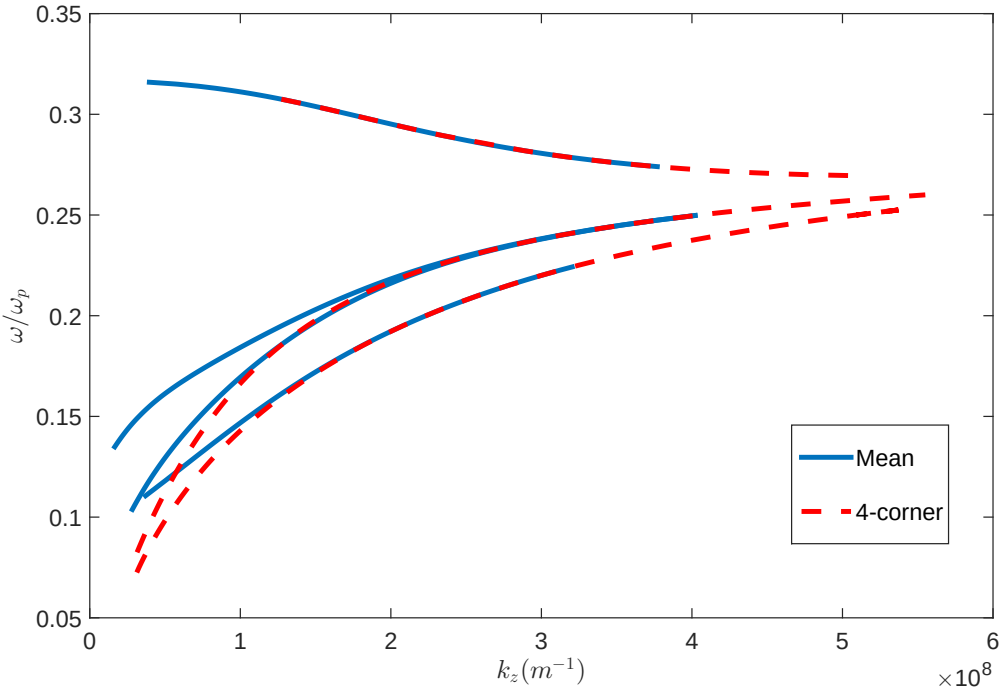
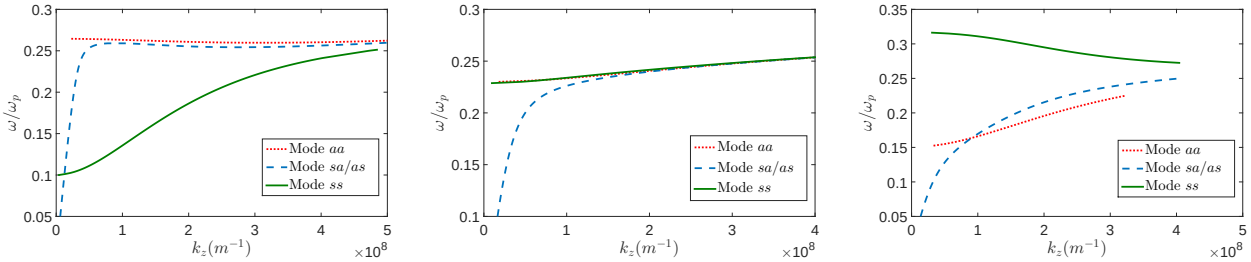


Figure 6: Comparison between the mean calculated with equation 2 and the four-corner excitation for the large nanorod array.



(a) $w = 8$ nm (b) $w = 16.3$ nm (c) $w = 25$ nm

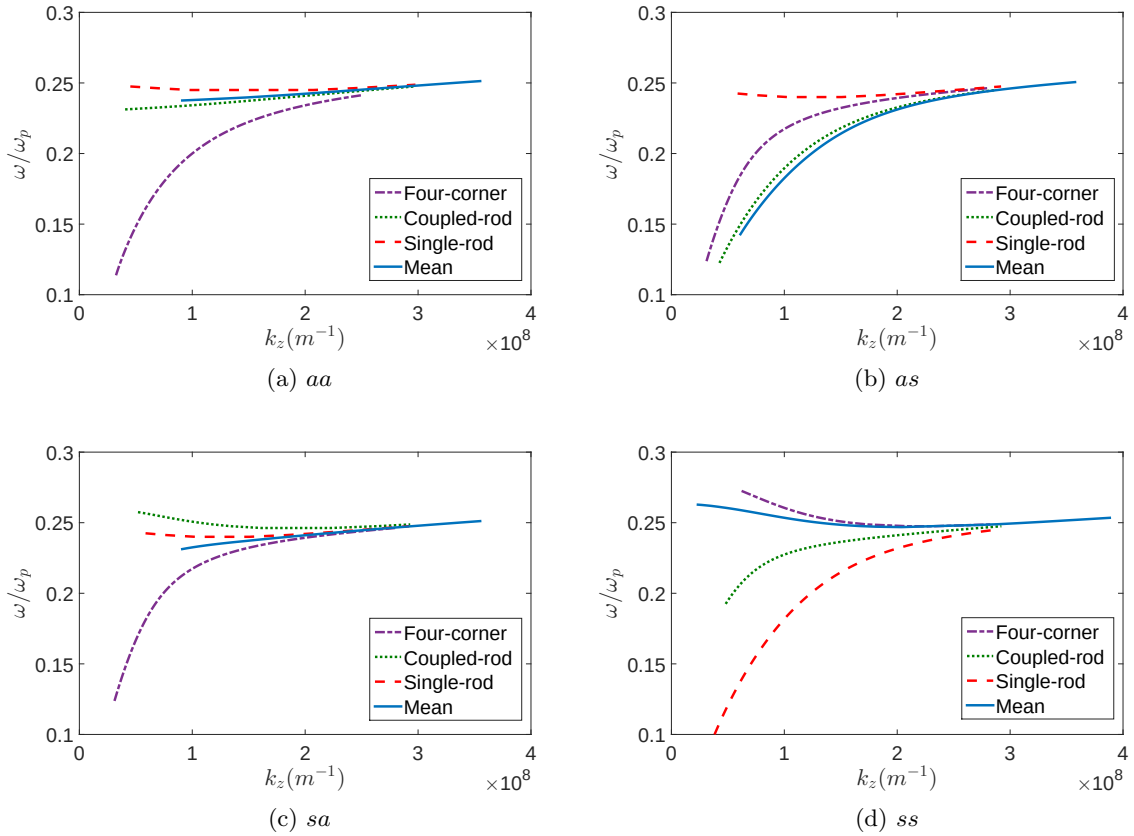
Figure 7: Dispersion at the center of the Brillouin zone for nanorod arrays of width (a) $w = 8$ nm (b) $w = 16.3$ nm (c) $w = 25$ nm.

Above $\omega = 0.246\ \omega_p$ all the modes approach the dispersion of the four corner structure. At medium size, the resulting elementary excitations thus depend on the symmetry and frequency range, which is a sign of similar coupling strength via metal-dielectric interfaces and through dielectric.

6. RECTANGULAR NANORODS

We now look for the case of asymmetry between the x and y directions by studying rectangular nanorods (Fig. 2d) with the width in the x direction much larger than in the y direction. Because the reduced Brillouin zone is now a square (Fig. 2e), we use equation 3 to calculate the mean and compare it to the adequate elementary excitation (Fig. 9).

Because the calculated mean corresponds very well with the coupled-rod dispersion, we conclude that the leading elementary excitation is therefore the coupled-rod structure and thus, the coupling is strong through the dielectric in the x direction and strong via sides of the nanorod in the y direction.



(a) aa (b) as

(c) sa (d) ss

Figure 8: Comparison between the mean calculated with equation 2 and the three possible elementary excitations for the medium size nanorod array. (a) aa mode. (b) as mode. (c) sa mode. (d) ss mode.

7. CONCLUSIONS

We can directly associate the dispersion of an array of square or rectangular metallic nanorods with the modes of simpler geometries. The particular simpler structure depends strongly on the size and shape of the nanorods and can be determined via the analysis method proposed in this paper.

We demonstrate that because of a strong coupling via the metal-dielectric interface (thus the sides of the nanorods) the dispersion of small square nanorod arrays originates from single-rod excitations. Similarly, because of strong coupling through the dielectric, large square nanorod arrays are associated with four-corner structures.

For the intermediate size regime, the elementary structure depends on the frequency and symmetry of the mode due to the similar strength of coupling via the metal sides and through the dielectric.

Finally, the rectangular nanorod (with one relatively large side) array dispersion originates from the coupled-rod excitation, because the coupling in the narrow direction is along the metal rod sides and through dielectric in the other direction.

In brief, one can understand the dispersion in arrays of metallic nanorods via their elementary excitations. The method presented in this paper can be applied to many other types of metamaterials.

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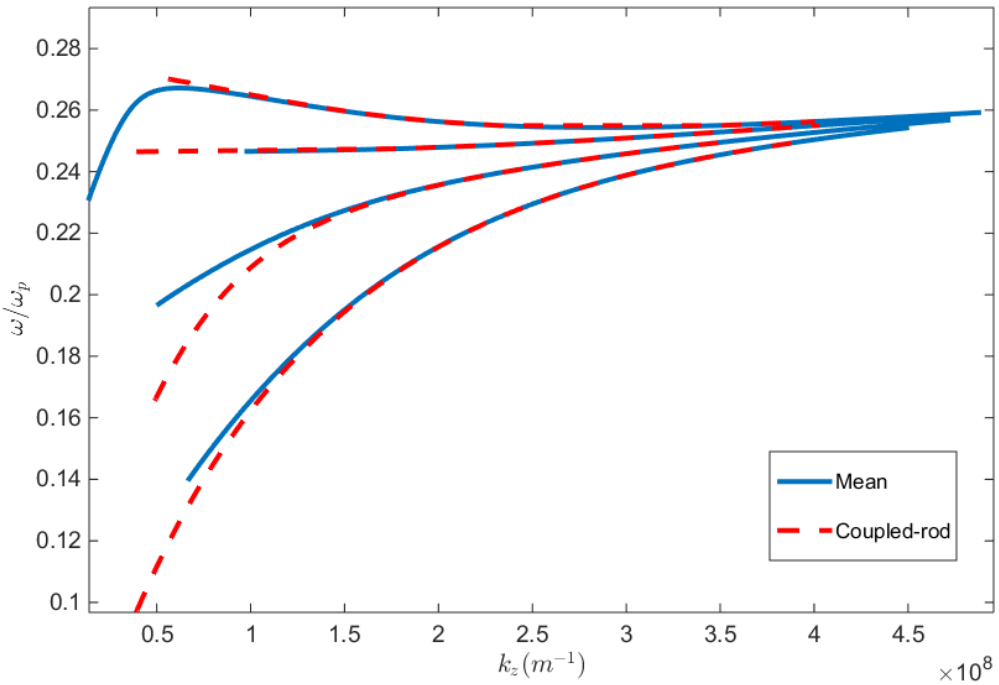

Figure 9: Comparison between the mean calculated with equation 3 and the coupled-rod excitations for the rectangular nanorod array.

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