Describing the dispersion of hyperbolic metamaterials by elementary excitation coupling

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Hyperbolic metamaterials are extremely anisotropic materials with iso-frequency surfaces shaped as hyperboloids, unlike natural materials. These metamaterials are interesting for many applications thanks to the large density of states and the extreme confinement of light they provide. We show that the dispersion of metamaterials made of square or rectangular metal nanorods in a 2D lattice can be understood via the coupling of elementary excitations, which often turn out to be the plasmons supported by the nanorod corners. Depending on the size of the nanorods, coupling occurs mainly through the dielectric or through the metal.

State of the art

Metamaterials have created a huge interest thanks to their extraordinary light control potential, impossible with natural materials [1, 2]. Among metamaterials, hyperbolic metamaterials (HMMs) caught the attention because of their extreme photonic density of states [3] and very large refractive index [4, 5], thanks to the anisotropy. HMMs are a particular case of an anisotropic medium where components of the diagonalized permittivity tensor are of opposite sign.

Classicaly, two types of structures are used to obtain the hyperbolic properties [6]: a periodic metal/dielectric multilayer structure (Fig. 1a) and an array of cylindrical metallic nanorods in a dielectric host (Fig. 1b).

In the case of the multilayer structure, effective medium theory (EMT) can be applied giving:

$$\varepsilon_{\parallel} = \frac{\varepsilon_m d_m + \varepsilon_d d_d}{d_m + d_d} \tag{1}$$

$$\varepsilon_{\perp} = \frac{\varepsilon_m \varepsilon_d (d_m + d_d)}{\varepsilon_m d_d + \varepsilon_d d_m} \tag{2}$$

with $\varepsilon_{\parallel}$ the permittivity in the direction parallel to the layers, $\varepsilon_{\perp}$ the permittivity in the direction perpendicular to the layers, ε_m and ε_d the permittivity of the metal and the dielectric, respectively, d_m and d_d the thickness of the metal and dielectric layers, respectively. The dispersion relation for extraordinary waves (TM polarisation) for such structures according to EMT is:

$$\frac{k_{\parallel}^2}{\varepsilon_{\perp}} + \frac{k_{\perp}^2}{\varepsilon_{\parallel}} = \frac{\omega^2}{c^2} \tag{3}$$

and for a regime where $\varepsilon_{\parallel}\varepsilon_{\perp} < 0$, the isofrequency surface is an open hyperboloid (Fig. 1c).

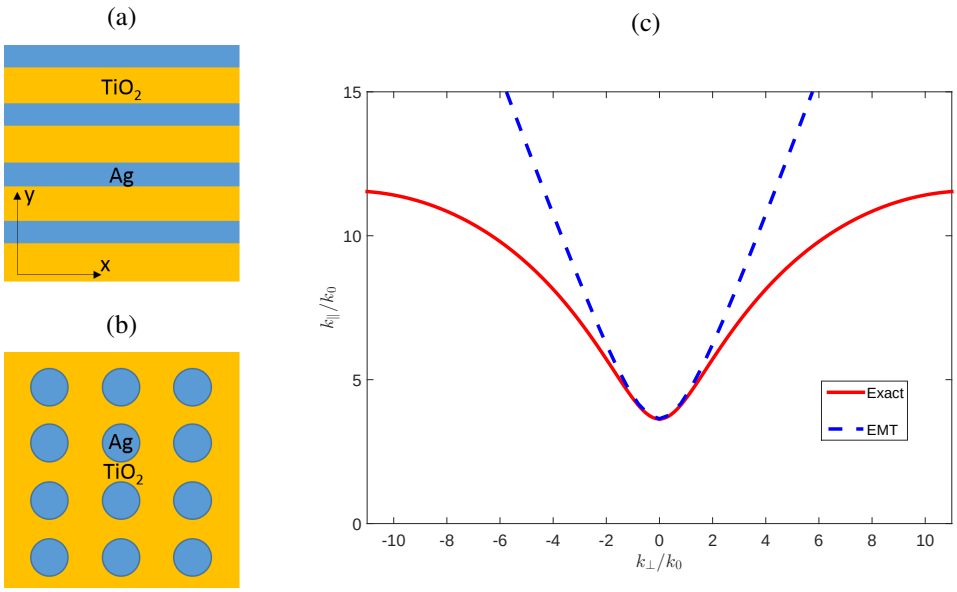

Figure 1: (a) HMM consisting of alternating periodic subwavelength layers of silver and TiO_2. (b) HMM consisting of on an array of cylindrical silver nanorods in a TiO_2 host. (c) Isofrequency contour for a multilayer HMM with d_{Ag} = 10 nm and d_{TiO_2} = 20 nm.

In 2013, Zhukovsky *et al.* shows the plasmonic origin of the hyperbolic properties in a multilayer HMM, so that the modes are explained as the coupling of short-range surface plasmon polaritons (SPPs) of each unit cell [7]. In 2011, Rosenblatt and Orenstein propose a method to describe the dispersion of multilayer HMMs as a competition between the coupling of gap modes (coupling of the surface plasmons at each metal/dielectric interface through the dielectric) and slab modes (coupling of the surface plasmons at each metal/dielectric interface through the metal) [8]. The purpose of this paper is to show an analogical demonstration for the more complicated 2D structures.

Analysis method

We numerically study the dispersion of arrays of silver (Ag) square and rectangular nanorods of various sizes in a TiO_2 host (Fig. 2a). We take the refractive index of TiO_2 n_{TiO_2} = 2.7 and a drude model for silver with $\omega_p = 1.26 \times 10^{16}$ Hz, where ω_p is the plasma frequency of silver. Contrary to the multilayer case were the simplest excitation possible is the SPP, the simplest excitation here is the plasmon carried by the corner of a nanorod. We fix the period of the array P = 30 nm, wich is much smaller than the wavelength in the regime analysed (from visible to near infrared). Four cases are examined: array of small (compared to the period) square nanorods with width w of the rod w = 8 nm, large square nanorod with w = 25 nm, medium size square nanorod with w = 16.3 nm and rectangular nanorod with w_x = 20 nm and w_y = 10 nm. There are three elementary excitations possible in this case, following through which medium the coupling between corners is stronger: a single rod (coupling mainly through the metal, Fig. 2b), 4 corners structure (coupling mainly through the dielectric, Fig. 2c) and coupled rods structure (coupling mainly through metal in one direction and dielectric in the other one, Fig. 2d).
To determine from which elementary excitation the dispersion of the array originates, we look which elementary excitation is near the center of each plasmonic band, mathemati-

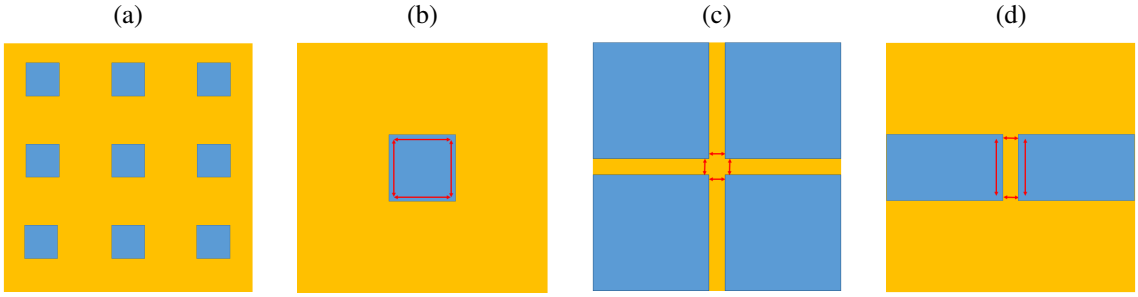

Figure 2: (a) Structure under study, array of square/rectangular nanorods. Elementary structures: (b) single rod, (c) 4 corner structure, (d) two semi-infinite coupled rods.

cally meaning that the elementary excitation is approximatively equal to the mean:

$$\omega_{elementary}(k_z) \approx \frac{\omega_{array}(\Gamma,k_z)+\omega_{array}(\mathrm{X}_1,k_z)+\omega_{array}(\mathrm{M},k_z)}{3} \tag{4}$$

for the array of square nanorods and

$$\omega_{elementary}(k_z) \approx \frac{\omega_{array}(\Gamma,k_z)+\omega_{array}(\mathrm{X}_1,k_z)+\omega_{array}(\mathrm{X}_2,k_z)+\omega_{array}(\mathrm{M},k_z)}{4} \tag{5}$$

for the array of rectangular nanorods, where $\omega_{elementary}$ is the frequency of the elementary excitation and ω_{array} the frequency of the array structure at the $\Gamma(k_x = k_y = 0)$, $\mathrm{X}_1(k_x = \frac{\pi}{P}, k_y = 0)$, $\mathrm{X}_2(k_x = 0, k_y = \frac{\pi}{P})$ and $\mathrm{M}(k_x = k_y = \frac{\pi}{P})$ points. The difference between the array of square and rectangular nanorods is that the symmetry between the x and y direction is broken for the rectangular nanorods and so $\mathrm{X}_1 \neq \mathrm{X}_2$.

Results

Contrary to the multilayer case, where only two different modes exist (a symmetric and an asymmetric one), the array of nanorods presents 4 different modes that can be symmetric or asymmetric in the x and y directions. We only present here the results for the mode symmetric in the x and y directions (Fig. 3) but the conclusions are the same for the four modes. We can see that the center of the plasmonic band corresponds very well with the single rod mode for the array of small nanorods (Fig. 3a) and thus, the coupling between the corners occurs mainly via the metal.

For the array of large nanorods however, the single rod is no more the elementary excitation that explains the dispersion, because the coupling occurs mainly through the dielectric, and thus the elementary excitation is the 4 corner structure mode (Fig. 2c).

The case of medium size nanorods is more complicated because the elementary excitation depends on the symmetry of the mode and on the frequency, meaning that at this regime of size the coupling through metal and dielectric is in the same order of magnitude and depends strongly on the frequency (Fig. 3c).

Finally, the center of the plasmonic bands for the rectangular nanorod case corresponds very well with the coupled rod excitations, meaning that the coupling occurs mainly through the metal in one direction and through the dielectric in the other one (Fig. 3d).

In conclusion, we have shown a method to understand the dispersion of an array of square or rectangular nanorods of any size, which opens the way to comprehend the dispersion of many types of metamaterials via their elementary excitations.

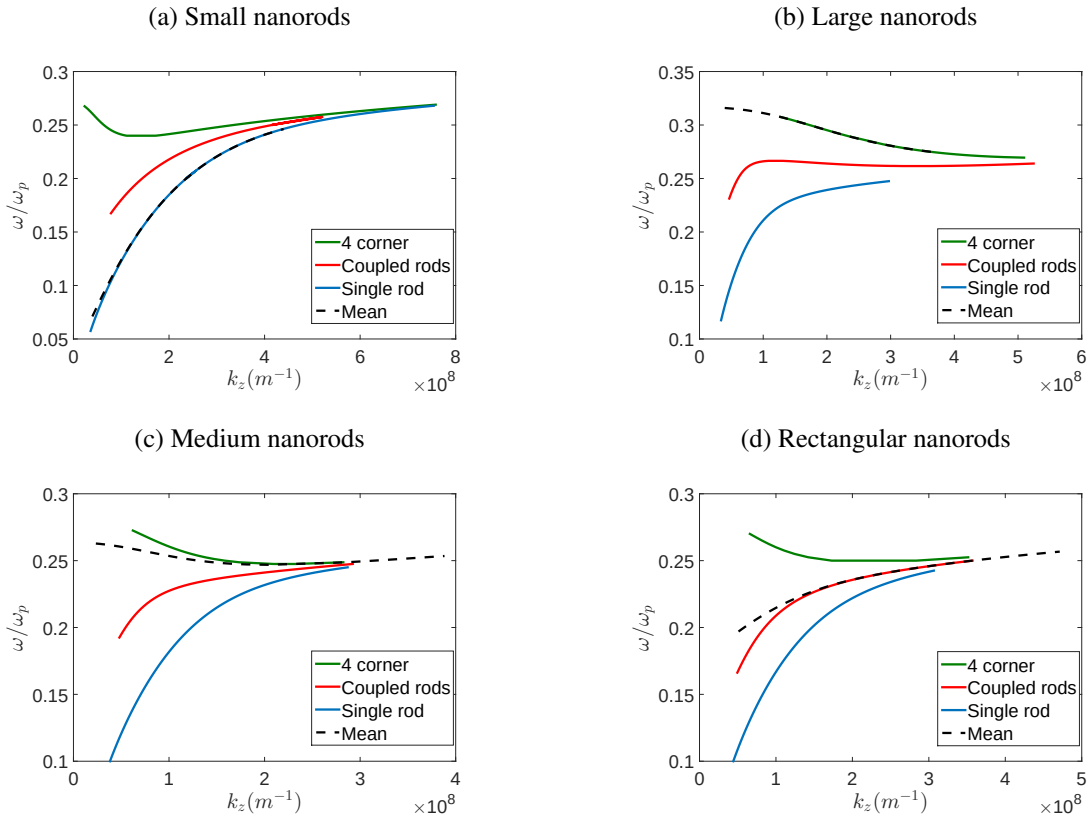

Figure 3: Comparison between the center of the plasmonic band (obtained with equation 4 or 5, black dashed curve) and the elementary excitations for the mode symmetric in the x and y directions.

Acknowledgments

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