Photonic Band Structure and Field Distribution for TE Polarization. High Plasmon Concentration in the Corners of Metallic Rods of a 2D Photonic Crystal

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Abstract— In this work we calculated the photonic band structure (PBS) of a square 2D photonic crystal (PC) made of square metallic rods embedded in air, considering a Drude type dielectric function without loss for different values of the rod plasma frequency, ω_p. The PBS was calculated for TE polarization in the Γ-X direction using the revised plane wave method (RPWM), considering the Li's rules for the product of two periodic functions. We found that the PBS presents flat bands below and above the surface plasmon frequency (SPF), and by means of the distribution of the square module of the magnetic component of the electromagnetic radiation, $|H_z|^2$, in the crystal unit cell, we found that these bands are related with the existence of plasmons in the surface of the rods, as it has been discussed and published in previous works. Besides these findings, we found a high concentration of the square module of the electric component of the electromagnetic radiation, $|E|^2$, close to the rod corners, which is a signature of the existence of localize surface plasmons, due to the geometry of the PCs structure. On the other hand, we found that $|H_z|^2$ presents a distribution which does not change in passing from the metallic regime to the dielectric one for frequencies close to ω_p, while $|E|^2$ is distributed only inside the rods for frequencies below ω_p, and essentially in the whole unit cell above this value.

1. INTRODUCTION

In recent years the study of photonic crystals (PCs) and their optical properties [1–3], aroused the interest of the scientific community, thanks to the discovery of the photonic band gaps present in these structures, that is, frequency ranges where the propagation of the electromagnetic field is prohibited, allowing the development of new technologies [4].

PCs are an arrangement of materials with different refraction index, which allow light behaviors not present in the bulk materials that form the PC. The photonic band structure (PBS) and the band gaps in the PCs depend on the difference between the refractive index of the components of the PC, their geometry disposition, and the filling fraction. The different studies on these structures rang from multiple slabs of different materials for 1D systems up to 3D structures [1–8], including fractal disposition of a dielectric material in air in a limited region of the space [9, 10]. Also, some studies are related to defects which modify the translation symmetry of PCs which allows the existence of high localized modes used in the construction of wave guides.

Maxwell equations are used to study the light behavior in PCs. To solve them several techniques have been developed such as plane waves, finite difference time domain (FDTD), revised plane wave method (RPWM), and others [11], and have been applied to several systems in order to study their optical response [12–14].

For PCs formed by dispersive materials it is possible to locate the incident radiation thanks to the existence of surface plasmon polaritons, that are related with the collective motion of coupled charges with the electromagnetic field [15].

Kusmiak et al. [12] studied a 2D system made of an arrange of parallel metallic rods in air using the plane wave method, reducing the PBS calculation to a standard eigenvalue problem. They show the existences of localized modes for TE polarization that must correspond to the interaction of the rod isolated excitations that overlap in the PC to form flat bands. This observation was corrected by Ito et al. [16], who presented a calculation based in a dipolar radiation implemented on the FDTD method to study the PBS, showing a strong distribution of the electromagnetic field on the surface of the rods, near to the resonant frequencies of a single rod under normal incidence for the electromagnetic radiation, that corresponds to the excitation of localized plasmon polariton in the metallic rod. Esteban Moreno et al. [17], demonstrated that the hypothesis by Ito et al. about the dipolar radiation for the excitation of surface localized modes in the crystal is not enough for another geometry of the rods, being necessary a generalization of the FDTD method using a set of dipoles in the unitary cell. It is important to note that the location shown by Ito et al., as well as the results obtained by Esteban Moreno et al., show that the field at the surface of the metal bars is distributed satisfying any of the symmetries of the metal cross section, also they show that the PBS for the circular cross section has bands with low dispersion below the surface plasmon frequency (SPF). These flat bands are distributed around frequencies which correspond to the resonant modes of the metal rods. Now that Esteban Moreno et al. also presents the study of a PC formed by bars with triangular cross section, showing the existence of flat bands above and below the SPF, demonstrating that the flat bands are distributed around the resonant modes of the rods, but the bands distribution above the SPF depends strongly on the geometry of the cross section of the rods.

In this work we study a 2D PC formed by an square arrangement of square metal rods embedded in air without dispersion in the materials. We calculate the PBS and some distributions of $|H_z|^2$ and $|E|^2$ in the unitary cell defined for the crystal using the RPWM method in order to elucidate the existence of surface plasmons in these systems.

2. THEORETICAL FRAMEWORK

We use the RPWM [18], for the calculation of the PBS of the PC proposed in the introduction. Considering square rods made of metallic material with dielectric function ϵ_m in a square lattice embedded in air, whose axes are parallel to z direction, it is possible to show that for TE polarization, $(\vec{H} = (0, 0, H_z), \vec{E} = (E_x, E_y, 0))$, and with a plane wave representations for the electrical and magnetic field, the Maxwell equations can be organized in the form

$$k_x \begin{bmatrix} [E_y] \\ [H_z] \end{bmatrix} = \frac{1}{k_0} \begin{bmatrix} -k_0\,[[G_x]] & k_0^2 - (k_y + [[G_y]])\,[[\epsilon_{xx}]]^{-1}\,(k_y + [[G_y]]) \\ k_0^2\,[[\epsilon_{yy}]] & -k_0\,[[G_x]] \end{bmatrix} \begin{bmatrix} [E_y] \\ [H_z] \end{bmatrix}, \qquad (1)$$

where $k_0 = \frac{\omega}{c}$ with ω the frequency of the radiation, and $[[G_{x(y)}]]_{G,G'} = G_{x(y)}\delta_{G,G'}$, are diagonal matrices of order N formed with the components of reciprocal lattice vector $\vec{G} = (G_x, G_y, 0)$. $[E_y]$ and $[H_z]$ are column vectors of order N constructed by the coefficients of the plane wave representation of the electrical and magnetic fields. k_x and k_y are the components of the radiation wave vector $\vec{k} = (k_x, k_y, 0)$ in the plane x-y.

The matrices $[[\epsilon_{xx}]]$, $[[\epsilon_{yy}]]$ are matrices of order N constructed following the Li's rules for the

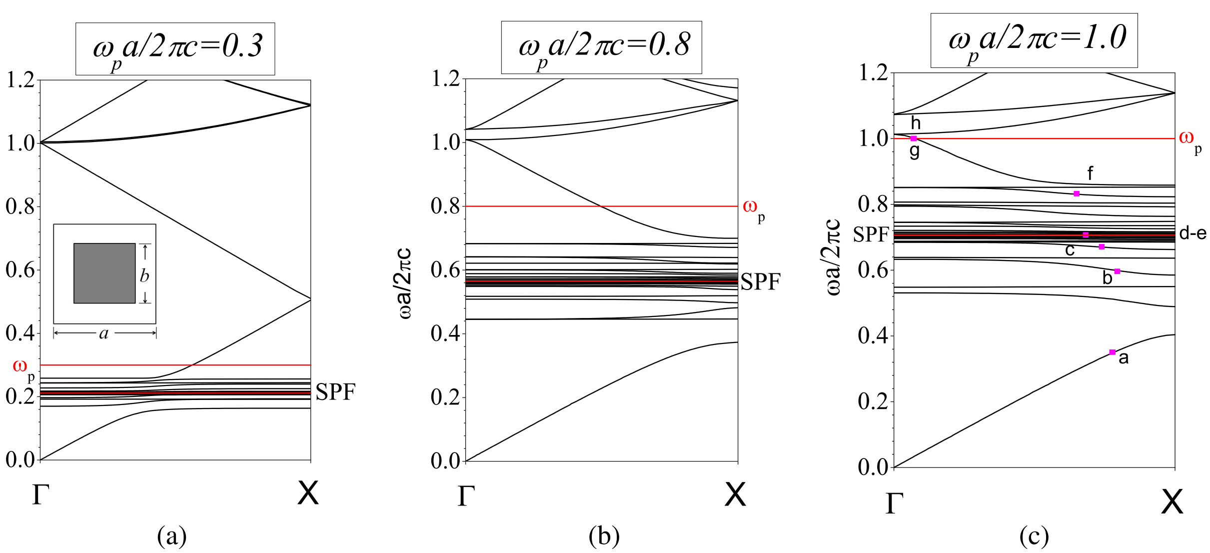

Figure 1: Photonic band structure for TE polarization in the Γ-X direction of a square lattice of square metallic rods embedded in air (inset in Fig. 1(a)), with $b/a = 0.25$, being a the lattice parameter and b the side size of the square rod. The value of plasma frequency is: (a) $\omega_p a/2\pi c = 0.3$, (b) $\omega_p a/2\pi c = 0.8$, (c) $\omega_p a/2\pi c = 1.0$. Red lines show the ω_p frequency and the value of the SPF. The purple marked squares a–h in Fig. 1(c) are to display $|H_z|^2$ and $|E|^2$ as it is presented in Fig. 2.

product of two periodic functions [19, 20]. In our case we have

$$[[\epsilon_{xx}]]_{mn,m'n'} = \frac{1}{a}\int_{-a/2}^{a/2} [[A_x^{-1}]]_{m,m'}\, e^{-i(n-n')g_y y} dy, \tag{2}$$

$$[[A_x]]_{m,m'} = \frac{1}{a}\int_{-a/2}^{a/2} \frac{1}{\epsilon} e^{-i(m-m')g_x x} dx, \tag{3}$$

where $g_i = |\vec{b_i}|$ are the elementary translation vectors of the reciprocal lattice, a is the lattice parameter and ϵ is a periodic function that takes the value of ϵ_m in the rods and is 1 in air. The coefficients of the matrix are relating the term $\vec{G} = m\vec{b}_x + n\vec{b}_y$ with $\vec{G}' = m'\vec{b}_x + n'\vec{b}_y$. A similar construction follows for $[[\epsilon_{yy}]]$.

The calculation of the PBS in Γ-X direction, that is with $k_y = 0$, is obtained solving the eigen values of Eq. (1).

3. RESULTS

By means of Eq. (1), we calculate the PBS of a 2D square PC made of square rods of metal embedded in air for three values of plasma frequency, which in practice corresponds to different

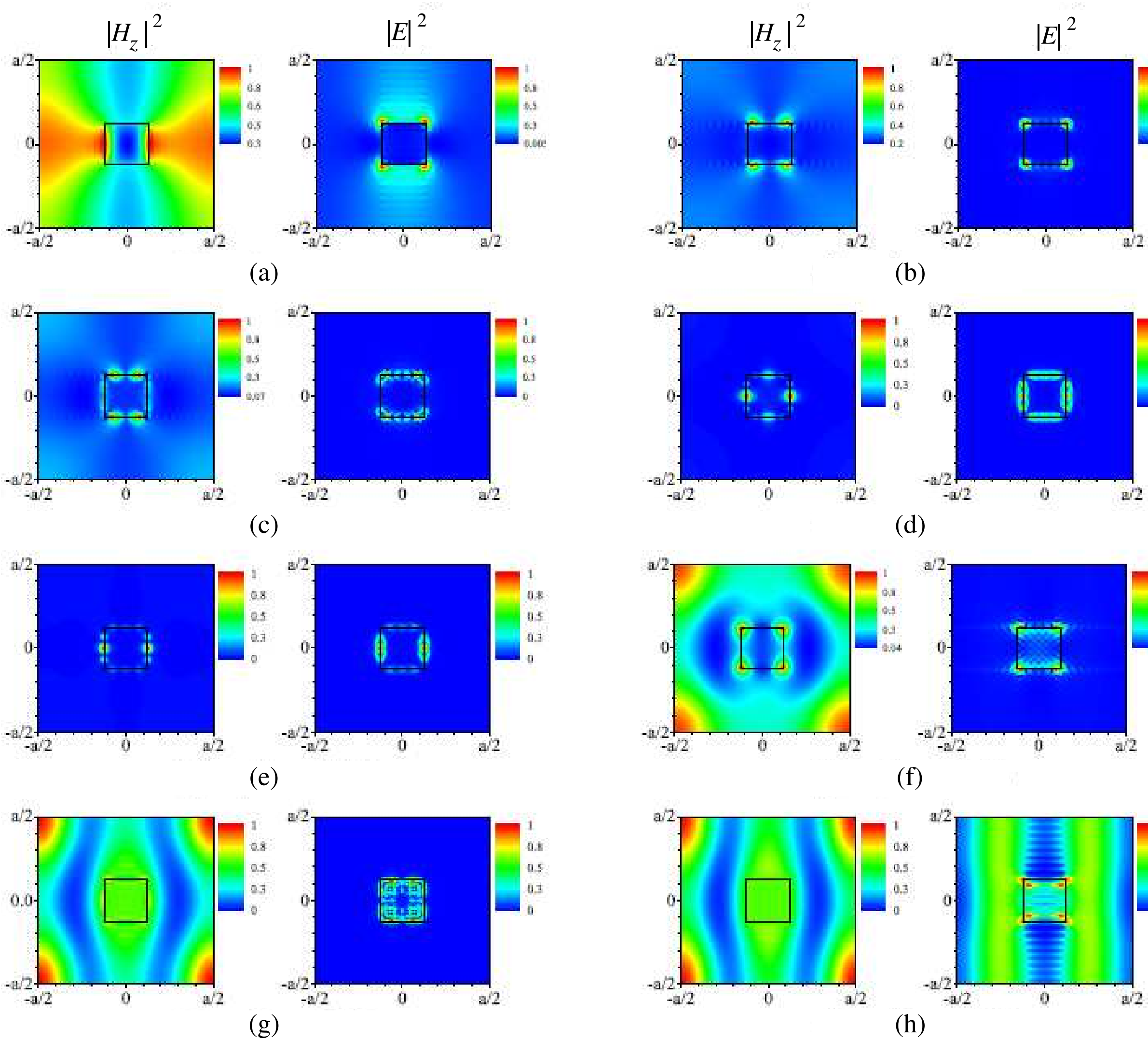

Figure 2: Some distributions of $|H_z|^2$ and $|E|^2$ in the unitary cell of a PC made of square metallic rods in air with $\omega_p a/2\pi c = 1.0$ and $b/a = 0.25$. The intensity distribution is in arbitrary units. (a) $\omega a/2\pi c = 0.361$, (b) $\omega a/2\pi c = 0.595$, (c) $\omega a/2\pi c = 0.670$, (d) $\omega a/2\pi c = 0.706$, (e) $\omega a/2\pi c = 0.708$, (f) $\omega a/2\pi c = 0.835$, (g) $\omega a/2\pi c = 0.999$, (h) $\omega a/2\pi c = 1.001$.

metals. We consider squares rods with $b/a = 0.25$, where b is the length of the square side and a is the lattice parameter. The dielectric function of the rod material is assumed as [21]

$$\epsilon_m = 1 - \frac{\omega_p^2}{\omega^2}, \tag{4}$$

where ω_p is the plasma frequency.

In Fig. 1, we observe the PBS characterized with flat bands localized below ω_p, behavior just reported by Ito et al. [16], due to the characteristic resonance frequencies associated with the existence of surface plasmons on the rod surface. Also, we found that for higher values of the ω_p, not only flat bands, but also new dispersive bands appear above the ω_p.

Figure 2 displays some field $|H_z|^2 - |E|^2$ distributions in the unitary cell for $\omega_p a/2\pi c = 1.0$. For low frequencies and in the dispersive band, Fig. 2(a), we observe that $|H_z|^2$ and $|E|^2$ are distributed outside the rod, and $|E|^2$ presents a strong concentration close to the corners of the rod, related with the movement of charge over the surface of the rod, but localized in their corners. On the other hand for higher frequencies, Figs. 2(b) and 2(c), show a high localization in the rod region, due to the smaller absolute values of the dielectric function of the metal, which promote the entering of radiation into the rod, while the distribution $|E|^2$ shows the formation of surface plasmons.

Figures 2(d) and 2(e), present the field distribution for higher and lower frequencies, close to the SPF, showing strong plasmon localization in the rod sides, in agreement with the low group velocity of radiation. For frequencies above the SPF, Fig. 2(f), the $|H_z|^2 - |E|^2$ distributions show the presence of radiation in the rod regions, because of the metal has the lower absolute value of the dielectric function. With respect to $|E|^2$ distribution, we observe that the field is highly concentrated in the corners. For frequencies below and above to ω_p, Figs. 2(g) and 2(h), present a similar $|H_z|^2$ distribution in the unitary cell, differently to the case for the $|E|^2$ distribution, which below ω_p forces the electric field to enter into the rod, due to the low absolute value of its refractive index, while for frequencies above ω_p the electric field is mainly distributed into the rod, but also with a strong presence in the air region. In these case, both materials present a positive refractive index, but the metallic rod is the material with the lower one, which makes the radiation to concentrate inside the rod.

4. CONCLUSION

In this work, using the RPWM we calculate the PBS in the Γ-X direction of a 2D square PC formed of square metallic rods embedded in air for the TE polarization. We found that the PBS of the PC depends markedly on the value of the ω_p, which modifies and shifts it to lower or higher frequencies. For all values of ω_p the PBS is characterized by the existence of flat bands below the plasma frequency related with the existence of localized surface plasmons in the rod surfaces, bands which are distribute around the SPF. By means of $|H_z|^2$ we encounter that for frequencies which make ϵ large negative in the rod region, the field is expelled out of the rods, behavior that also occurs for $|E|^2$, with a strong concentration of the field in the corners of the rods, due to the movement of charge in the metal caused by the electric field. For frequencies very close to the SPF we observe a strong localization of the fields on the surface of the rods. As $|\epsilon|$ decreases in the metal we encounter a distribution that is characterized by the existence of localized surface plasmons. On the other hand for frequencies between the SPF and ω_p, the field enters inside the rod, being more evident in the $|E|^2$ distribution just below ω_p. Above ω_p we found the common behavior of localization of the radiation, presenting a discontinuity of $|E|^2$ across the surface of the rod due to its discontinuity in the metal surface.

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