Enhancement of the Purcell Effect by the Wire Metamaterials Formed by the Hexagonal Unit Cells

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Abstract: The dependence of the Purcell factor on nanowire metamaterial geometry was analyzed. Calculations made about the Purcell factor in realistic composites, operating at an optical spectral range, are provided. We applied a metamaterial, aiming to mitigate the negative effects of absorption in metals on the Purcell effect in nanowire structures. A nanowire metamaterial was treated as an anisotropic composite in the long-wavelength limit. We investigated the mode patterns of the surface waves, propagating at the boundary separating such a structure and a dielectric material, along with the position of the peak in the local density of states, for the various filling factors of the periodic structure. By calculating the frequency dependence of the Purcell factor, we showed an increase in the peak value in comparison with the conventional plasmonic structure in the (1–100 THz) frequency range. Moreover, an optimal set of the parameters, needed to obtain the two topological transitions in the frequency range under investigation, is proposed.

Keywords: Purcell factor; metamaterial; nanowire

1. Introduction

Nanowire metamaterials, which drastically affect fundamental physics and practical applications, have attracted significant attention over the years. These nanowire metamaterials open wide avenues from which hyperbolic dispersion can be achieved [1]. Considerable scientific interest has been sparked due to the reason that conventional geometry (such as nanowire arrays [2] and metal-dielectric nanostructures [3,4]), allows for the achievement of hyperbolic metamaterial functionality. It is worthwhile mentioning that one may tailor the mode patterns of surface plasmons in an extraordinary way, by means of a one-dimensional, metal-based, corrugated structure that represents a simple metasurface, possessing almost realistic geometry [5].

In doing so, the nanowire composite is a unique example of a hyperbolic medium that opens wide avenues for the high density of states [6–8]. A broadband increase in the density of photonic states, in comparison with vacuum by the factor of the order \((\lambda/a)^2\), where \(\lambda\) is the wavelength and \(a\) is the lattice period [9], stands as a particular feature of the wire medium. This causes the remarkable enhancement of the light–matter interaction outcomes; the former includes the spontaneous emission (the Purcell effect) [10–12], Vavilov–Cherenkov radiation [13,14], and heat transport [15].

Our goal was to perform a comprehensive analysis that accounted for the finite dielectric constant of the wires. The work is organized in the following way: (1) our theoretical model is presented in Section 2; (2) the study of the eigenmode dispersion of the composite is presented in Section 3. Additionally, the analytical results for the Purcell factor are considered. The discussion about whether the Purcell factor is achievable in different cases is also summarized.
2. Methods

Figure 1 displays the boundary separating the structure under investigation, based on the nanowire composite [16] and the dielectric. It is worthwhile mentioning that each wire only interacts with another as a macroscopic source. The wires characterized by the permittivity $\varepsilon_m$ were implanted in a host media with the permittivity $\varepsilon_d$. It is worthwhile mentioning that the unit cell of the metamaterial possessed a hexagonal shape. The former arrangement was possible through utilizing the DNA origami nanostructures to guide the higher-order arrangement of the nanowires in a controlled and programmable manner [17]. In doing so, the structure under consideration stands as a promising tool for further applications.

![Figure 1](image_url)

**Figure 1.** A view of the boundary, splitting up the nanowire composite and dielectric medium (a); a hexagonal unit cell (b).

The dielectric properties of the nanowire metamaterial, in different directions, were assessed by means of the Maxwell–Garnett effective medium approximation [1], and were derived by starting from Schrodinger’s wave equation:

$$\varepsilon_{\perp} = \frac{\varepsilon_m(1 + \rho) + \varepsilon_d(1 - \rho)}{\varepsilon_m(1 - \rho) + \varepsilon_d(1 + \rho)}$$

(1)

$$\varepsilon_{\parallel} = \varepsilon_m\rho + \varepsilon_d(1 - \rho)$$

(2)

Here, $\rho$ is the metal filling fraction factor, calculated as follows:

$$\rho = \frac{\text{nanowire area}}{\text{unit cell area}}$$

(3)

The Drude model was adopted, with the aim of having a deeper insight into the particularities of the surface waves, and to describe the metal (i.e., silver). In doing so, permittivity was expressed as $\varepsilon_m(\omega) = \varepsilon_{\infty} - \frac{\omega_p^2}{\omega^2 + \delta^2}$. The properties were found by matching this permittivity function to a particular frequency range in the bulk material [18]. It was concluded [19] that for the silver, the values of $\varepsilon_{\infty} = 5$, $\omega_p = 9.5eV$, $\delta = 0.0987eV$ gave us a reasonable fit. By making the assumption that the metamaterial unit cell had a hexagonal form, we determined the metal filling fraction ($\rho$). These calculations were affected by the estimates of the wires’ diameters ($d$), and the spacing ($S$), as follows [20]:

$$\rho = \frac{\pi d^2}{2 \sqrt{3} S^2}$$

(4)

Based on the presented assumption, it was worthwhile deriving a dispersion relation, with the aim of having a deeper insight into the mode patterns propagating at the interface, between the anisotropic media and dielectric. To have a deeper insight into the physical effects, it was particularly important to
obtain a single surface mode by estimating the tangential components of the electric and magnetic fields at the boundary [21]:

\[
\beta = k \left( \frac{(\varepsilon_d - \varepsilon_\parallel)\varepsilon_d\varepsilon_\perp}{\varepsilon_d^2 - \varepsilon_\perp \varepsilon_\parallel} \right)^{1/2}
\]

(5)

where \( k \) is the wavenumber being the absolute value of the wavevector in the vacuum, and \( \beta \) is the component of the wavevector parallel to the interface.

By substituting Equations (1), (2), and (5), we arrived at:

\[
\beta = k \left( -\frac{\varepsilon_d\chi(\varepsilon_d - \varepsilon_m\rho + \varepsilon_d(\rho - 1))}{(\varepsilon_d(\rho + 1) - \varepsilon_m(\rho - 1))(\varepsilon_d^2 + \frac{(\varepsilon_m - \varepsilon_d(\rho - 1))\chi}{\varepsilon_d(\rho + 1) - \varepsilon_m(\rho - 1)})} \right)^{1/2}
\]

(6)

\[
\chi = (\rho - 1)\varepsilon_d^2 - \varepsilon_m(\rho + 1)\varepsilon_d
\]

We noted that Equations (5) and (6) are valid only under the condition of the surface confinement, which can be presented in the following form:

\[
\begin{cases}
  (k^2 - \beta^2/\varepsilon_\parallel)\varepsilon_\perp < 0 \\
  (k^2 - \beta^2/\varepsilon_\parallel)\varepsilon_\perp < 0
\end{cases}
\]

(7)

It is worthwhile noting that if \( \rho = 1 \), we arrive at the conventional equation for the propagation of the surface plasmon polaritons on the metal/dielectric interface, presented below as:

\[
\beta = k \left( \frac{\varepsilon_m \varepsilon_d}{\varepsilon_m + \varepsilon_d} \right)^{1/2}
\]

(8)

The formula for the Purcell factor is as follows [22]:

\[
P_F = \frac{\varepsilon_\parallel}{4\sqrt{\varepsilon_\perp}} + 3\frac{\sqrt{\varepsilon_\perp}}{4}
\]

(9)

3. Results

In the following, we will demonstrate how the proposed structure can be used to control the properties of the metamaterial, mode patterns of a surface plasmon, and value of the Purcell factor.

It is worthwhile examining the resonance of the perpendicular permittivity. The frequency dispersion of \( \varepsilon_\perp \) is shown in Figures 2 and 3. Due to the low level of losses, the real part of \( \varepsilon_\perp \) changed the sign of the resonance. It is worthwhile noting that the regime \( \varepsilon_\perp = 0 \) facilitated the second topological transition, observable for \( d = 20, 30, \) and \( 40 \) nm but not for the case \( d = 10 \) nm. It should be mentioned that the resonance of the Purcell factor corresponded to the topological transition [23]. We also took into account the parallel component of the effective permittivity, due to the reason that the Purcell factor of a highly anisotropic metamaterial is defined by the factor \( \varepsilon_\parallel/\varepsilon_\perp \). Figures 2 and 3b show \( \varepsilon_\parallel \) versus the frequency.
Figure 2. (a) Dependences of the real parts of the perpendicular and parallel permittivity components, upon frequency of the silver nanowire metamaterial. (b) Dependence of the imaginary part of the perpendicular permittivity component upon frequency. $S = 70$ nm.

Figure 3. (a) Dependences of the real parts of the perpendicular and parallel permittivity components, upon frequency of the silver nanowire metamaterial. (b) Dependence of the imaginary part of the perpendicular permittivity component, upon frequency. $d = 30$ nm.

The surface plasmon polariton dispersion, calculated according to Equation (6), is shown in Figures 4 and 5. For comparison, the mode patterns of conventional surface waves propagating at the interface, separating the metal and dielectric, are also shown. It is of significant importance to mention that the plasmon associated with an ordinary wave was proven to be more effective in reducing the peak frequency of the local density of states (LDOS). It is obvious that by varying the filling factor, one can tune the peak frequency to any wavelength.
was very good. In doing so, the dispersion curves were approaching the conventional surface plasmon polaritons curve, in the case of the increase in $d$.

It is worthwhile noting that it might be found with the Purcell factor of the frequency in Figure 6, that the maxima of the Purcell factor were dramatically affected by the geometry of the composite.

It should be mentioned that the agreement between the results we obtained using different methods (Figures 4a and 5a) and the result with a rigorous calculation (the full wave method) is presented in Figure 4a for the case of $d = 10$ nm. The results we obtained from the full wave method are demonstrated with the blue markers.

Figure 4. Mode patterns of the surface waves at the interface of metamaterial and dielectric ($\varepsilon_d = 11.8$). $S = 70$ nm. Dependencies of the real (a) and imaginary (b) parts of the propagation constant, upon frequency.

Figure 5. Mode patterns of the surface waves at the interface of metamaterial and dielectric ($\varepsilon_d = 11.8$). $d = 30$ nm. Dependencies of the real (a) and imaginary (b) parts of the propagation constant, upon frequency.

It can be observed, in Figures 4 and 5, that if $\rho \rightarrow 1$, Re($\beta$) (Figures 4a and 5a) and Im($\beta$) (Figures 4b and 5b) are approaching the dispersion of the conventional surface plasmon polaritons, propagating at the metal/dielectric boundary. It is worthwhile mentioning that a comparison of the result with a rigorous calculation (the full wave method) is presented in Figure 4a for the case of $d = 10$ nm. The results we obtained from the full wave method are demonstrated with the blue markers. It should be mentioned that the agreement between the results we obtained using different methods was very good. In doing so, the dispersion curves were approaching the conventional surface plasmon polaritons curve, in the case of the increase in $d$. The same tendency can be observed in Figure 5a, in the case of the decrease in $S$.

The determined estimates of the Purcell factor are presented in Figure 6. It can be observed in Figure 6a that the Purcell factor was increased by increasing the diameter of the nanowires. Moreover, it can be clearly observed in Figure 6b that the Purcell factor was increased by decreasing the distance between the nanowire. In doing so, it can be clearly observed, by displaying the Purcell factor versus the frequency in Figure 6, that the maxima of the Purcell factor were dramatically affected by the geometry of the composite. It is worthwhile noting that it might be found with the Purcell factor
of an infinite wire metamaterial. Two amplitudes of the Purcell factor were located and kept for a
different geometry of the sample. Moreover, the Purcell factor enhancement was dramatically affected
by replacing the host medium of the wire metamaterial with a vacuum, as seen in Figure 6.

It can be observed in Figure 6a that a stronger resonance was caused by the growth in the radius
of the wires. It is worthwhile noting that, in this case, the lattice constant was fixed. Figure 2b
demonstrates the maximum in the lossy factor, $\text{Im}(\varepsilon_\perp)$, occurring at a frequency that was, to some
extent, lower than that of the band, in which $\text{Re}(\varepsilon_\perp)$ was negligible. Consequently, the growth in the
diameter of the wires ($d$) gave rise to the second resonance of the Purcell factor. It is worthwhile noting
that the second topological transition might have been lost by decreasing the distance between the
nanowires. Thus, in a predetermined lattice constant, there might be the best possible estimate for the
nanowire radius. Thus, Figure 6 demonstrates the optimal sets of the parameters that aim to achieve
two topological transitions in the investigated frequency range. It is worthwhile noting that Figure 6
also demonstrates a comparison in the results obtained for the host medium being either dielectric or
air. The decrease in the Purcell factor can be observed in the case of the air host medium, due to the
higher absorption and penetration of the electric field in the metamaterial.

The values of the Purcell factor for a conventional interface plasmon have also been demonstrated.
Figure 7 presents the dependence of the maximum value of the Purcell factor versus the filling ratio.
Lowering the LDOS peak frequency towards the low-absorption range was proven to be effective. The
value of the Purcell factor can be easily increased ten-fold. Importantly, a decrease in the value of the
filling factor increased the value of the Purcell factor for an ordinary plasmon. For the very small
values of the filling ratio, the maximum Purcell factor approached zero, as there can be no surface
plasmon on a dielectric/dielectric boundary. An increase in the filling ratio caused a decrease in the
Purcell factor.

(a) 

(b) 

Figure 6. Dependence of the Purcell factor upon frequency. (a) $S = 70$ nm; (b) $d = 30$ nm.
4. Conclusions

The resonances of the Purcell factor correspond to the topological transitions. It is worthwhile noting that we have chosen the optimal geometry of the nanowire metamaterial, aiming to achieve two topological transitions in the investigated frequency range. The obtained results provide fertile ground for broadband and strong radiation enhancement. The former is applicable in optical nanosensing, and in the radiative cooling of tiny bodies. Plenty of the described results have been achieved for nanowires made of silver. However, these findings might be similarly observed in the cases of other polaritonic materials.

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