# Angular and positional dependence of Purcell effect for layered metal-dielectric structures

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## Abstract

We study the angular dependence of the spontaneous emission enhancement of a dipole source inserted into a layered metal-dielectric metamaterial. We analyse the dependence of Purcell effect from the position of the dipole in the layered hyperbolic media. We analyse the impact of the complex structure of eigenmodes of the system operating in hyperbolic regime. We have shown that the spontaneous emission rate of the dipole emitter depend on its position, which mainly affect the interaction with Langmuir modes.

Keywords: Purcell factor; metamaterials; metal-dielectric nanostructures.

#### 1. Introduction

Periodical metal-dielectric structures have attracted great scientific attention as an application for engineering the spontaneous emission. Such structures are also classified as one-dimensional photon crystals, are generally known as a simple realization of the metamaterials [1]. Metamaterials have attracted great scientific interest over the past decade due to their special optical properties emanating primarily while operating in hyperbolic regime. According to the effective-medium approach the isofrequency surface of such systems is hyperbolic, when the principal components of the effective permittivity tensor  $\varepsilon_{eff}$  of the diagonal form [2]:

$$\varepsilon_{eff} = \begin{pmatrix} \varepsilon_{\perp} & 0 & 0\\ 0 & \varepsilon_{||} & 0\\ 0 & 0 & \varepsilon_{||} \end{pmatrix},$$
(1)

are opposite in sign:  $\varepsilon_{||}\varepsilon_{\perp} < 0$ . Where components along  $(\varepsilon_{||})$  and across  $(\varepsilon_{\perp})$  the optical axis, depending on permittivity and thickness of metal and dielectric layers, are given by:

$$\varepsilon_{\perp} = \frac{(d_m + d_d)\varepsilon_d\varepsilon_m}{d_m\varepsilon_d + d_d\varepsilon_m}, \qquad \varepsilon_{||} = \frac{d_m\varepsilon_m + d_d\varepsilon_d}{d_d + d_m}.$$
<sup>(2)</sup>

The dispersion relation of metal-dielectric metamaterials is given by:

$$\frac{k_x^2 + k_y^2}{\varepsilon_{||}} + \frac{k_z^2}{\varepsilon_{\perp}} = \left(\frac{\omega}{c}\right)^2.$$
<sup>(3)</sup>

The concept of the enhancement of the spontaneous emission of a dipole in a cavity is known as the Purcell effect, first proposed by Purcell in 1946 [3] within the framework of nuclear magnetic resonance. This effect is described by the Purcell factor, defined by the ratio between the probability of spontaneous emission of a dipole inserted into a resonant cavity to that in a free space. The origin of the enhancement of the spontaneous emission can be demonstrated according to the Fermi Golden rule. The radiative decay rate  $1/\tau$  in a homogeneous lossless medium is defined by:

$$\frac{1}{\tau} = \frac{2\pi}{h} \sum_{\boldsymbol{k},\sigma} |\langle f | H_{int}(\boldsymbol{k},\sigma) | i \rangle|^2 \,\delta(h \,\omega_{\boldsymbol{k},\sigma} - h\omega) \tag{4}$$

where  $\langle f | H_{int}(\mathbf{k}, \sigma) | i \rangle$  is the matrix of the perturbation between the initial  $|i\rangle$  and final  $|f\rangle$  states, with the transition energy  $h\omega$  and the photon emission  $(\mathbf{k}, \sigma)$ , where  $\mathbf{k}$  is the wave vector and  $\sigma$  is polarization. It was illustrated that the density of photonic states in metamaterials operating in hyperbolic regime diverges [4], affording an enhancement of the spontaneous emission [5].

Recently appeared theoretical estimations of the ultra-high enhancement of the spontaneous emission rate of the dipole embedded in the metal-dielectric metamaterials [5,6] or periodic dielectric [7] nanostructures are very interesting, providing a means to engineer many fascinating applications. These results deserve more careful consideration, particularly, it is interesting to study the angular dependence of the Purcell factor and to analyse the impact of the complex eigenmodes of such system. The aim of this work is to analyze how the spontaneous emission rate depends on the position of the dipole source in layered metal-dielectric structures.

#### 2. Theory

We study the Purcell effect for a point dipole emitter embedded in the central layer of the HMM system. This effect is described by the Purcell factor, which in the broad sense is defined by the ratio between lifetimes of spontaneous emission of a point light source in the vacuum to that inserted into a resonant cavity. The spontaneous emission in the vacuum is given by

$$\Gamma_0 = \frac{k_0^3 \mu^2}{3\pi\varepsilon_0 \hbar} \tag{5}$$

In a layered structure waves with two polarizations can independently propagate: transverseelectric (TE)-polarized and transverse-magnetic (TM)-polarized (illustrated schematically on figure 1). Therefore it is interesting to study the contribution to the Purcell effect in a symmetric multilayer stack separately for TE and TM polarized incident light with respect to different incident angles. We assume that the dipole-source is enclosed between two identical mirrors formed by periodical structures. Therefore the system can be treated as a cavity, and to calculate the Purcell effect we apply an approach based on the quantum theory of the spontaneous emission (SpE) [8], and the spontaneous emission of a dipole moment  $\mu$  is given by

$$\Gamma_{n}^{j} = \frac{k}{8\pi^{2}\varepsilon_{0}\hbar} \Big( |\{ \mathbf{E}(\mathbf{k}_{+},j)t_{1,j} + \mathbf{E}(\mathbf{k}_{-},j)t_{1,j}r_{2,j}\exp[ik(d-2z_{0})\cos\theta]\} \boldsymbol{\mu}||^{2} + |\{ \mathbf{E}(\mathbf{k}_{-},j)t_{2,j} + \mathbf{E}(\mathbf{k}_{+},j)t_{2,j}r_{1,j}\exp[ik(d+2z_{0})\cos\theta]\} \boldsymbol{\mu}||^{2} \Big) / D_{j}^{2}$$
(6)

where  $k_+$  and  $k_-$  indicate the wave-vector, for a wave outgoing on the right of the cavity (z>0), and for a wave outgoing on the left of the cavity (z<0). Polarization is indicated by index *j*: which is s - for TE and p - for TM polarisation. Subscript *n* indicate the dipole orientation,  $z_0$  is the z coordinate of the dipole position.

$$D_i = 1 - r_{1i} r_{2i} \exp(2ikd\cos\theta) \tag{7}$$

where indexes 1 and 2 correspond to left and right mirror, respectively. The complex reflection  $r_{s,p}$  and transmission  $t_{s,p}$  coefficients through layered media were calculated for each polarization by applying the transfer matrix method (TMM) [9] which provides accurate and reliable estimations of optical parameters of layered structures depending on the incidence angle  $\theta$ . And the Purcell factor is given by:

$$\mathbf{F}_p = \Gamma_n^j / \Gamma_0 \tag{8}$$

Hyperbolic metamaterial systems have complex structure of eigenmodes. The enhancement of spontaneous emission occurs when the emitted frequency is resonant with modes of the structure. To understand the contribution of each mode it is advisable to study independently two orientations of the dipole: perpendicular and parallel (subscripts  $\perp$  and  $\parallel$ ) to the interface of layers, and for each case to consider the contribution of TE and TM polarizations respectively. When the dipole is perpendicular to layers, for TE polarization the product of  $E_y$  component of electric field vector and the dipole is zero, therefore only TM polarization contribute to Purcell factor, which is given by:

$$F_{\perp}^{TM} = \frac{\Gamma_{\perp}^{TM}}{\Gamma_0} = \frac{3n_c^3}{8} (1 - \cos\theta) \{ \left| t_{1,p} \right|^2 |1 - r_{2,p} \exp[ik(d - 2z_0)\cos\theta]|^2 + \left| t_{2,p} \right|^2 |1 - r_{1,p} \exp[ik(d + 2z_0)\cos\theta]|^2 \} / D_p^2$$
<sup>(9)</sup>

where  $n_c$  is the refraction coefficient of the central layer, where dipole is placed. For the parallel case we can assume with no loss of generality that dipole is parallel to the *x* axis. For TE polarization the Purcell factor is given by:

$$F_{\parallel}^{TE} = \frac{\Gamma_{\parallel}^{TE}}{\Gamma_0} = \frac{3n_c^3}{8} \{ \left| t_{1,s} \right|^2 |1 + r_{2,s} \exp[ik(d - 2z_0)\cos\theta]|^2 + \left| t_{2,s} \right|^2 |1 + r_{1,s} \exp[ik(d + 2z_0)\cos\theta]|^2 \} / D_s^2$$
(10)

For TM polarization the Purcell factor is given by:

$$F_{\parallel}^{TM} = \frac{\Gamma_{\parallel}^{TM}}{\Gamma_0} = \frac{3n_c^3}{8} \{ \left| t_{1,p} \right|^2 |1 + r_{2,p} \exp[ik(d - 2z_0)\cos\theta]|^2 + \left| t_{2,p} \right|^2 |1 + r_{1,p} \exp[ik(d + 2z_0)\cos\theta]|^2 \} (\cos\theta / D_p)^2$$
(11)



Figure 1. A schematic structure of the stratified metamaterial formed by metal and dielectric layers with a dipole source embedded in the central dielectric layer, showing  $\perp$  and  $\parallel$  orientations of dipole  $\mu$  and polarizations of propagating waves.

### 3. Results and discussion

We study the angular dependence of the enhancement of the spontaneous emission of the dipole source embedded in the layered metamaterial, shown schematically in figure 1, constructed as a periodic structure by alternating metal and dielectric layers. In our model as metal we consider silver, which is described by the Drude model:  $\varepsilon_m = \varepsilon_{\infty} - \frac{\omega_p^2}{\omega(\omega + i\gamma)}$ , which was fitted to a particular frequency range of the Johnson and Christy experimental data [10] with the plasma frequency  $\omega_p \approx 8.98$  eV,  $\varepsilon_{\infty} \approx 4.96$  and the damping coefficient  $\gamma$ =0.018 eV. The permittivity of dielectric layers  $\varepsilon_d$  is equal to unity. We consider equal thickness of silver and dielectric layers  $d_m = d_d$ =30 nm.

To study how the Purcell factor depends on the position of the dipole in the system, we compare the results calculated for a dipole located at certain points. Particularly we locate the dipole in the central dielectric layer with thickness  $d_c = 30$  nm at the following two distances from the left mirror of the system: a) half of the core layer  $\mu_{point} = \frac{d_c}{2}$  and b) near the boundary of the metal and dielectric  $\mu_{point} = \frac{d_c}{60}$ .

We present results of the Purcell factor simulation as a function of incident angle  $\theta$ , evaluated for a range of frequencies, in figures 2-4. The system under consideration is characterized by complex structure of eigenmodes, to understand their contribution to the spontaneous emission rate we calculate the Purcell factor separately for different types of polarization of waves and parallel and perpendicular orientations of the dipole.

When the dipole is perpendicular to layers the Purcell factor, calculated by Eq. 9 for TM polarization, is presented in figure 2. As was presented in [8] the spontaneous emission can be enhanced when the dipole interact with the mode structure of the system. Electromagnetic waves in layered metal-dielectric structures addressed in details in [11,12], particularly, it was shown that volume, surface, and Langmuir waves can propagate in such layered structures. From our results we can see an enhancement of spontaneous emission when the frequency is resonant with volume, surface and Langmuir modes indicated in figure 2.

There are two poles, which divide the studied frequency range to regions where propagation of waves particular is dominant. First at the frequency, when the condition Real( $\varepsilon_m(\omega_{1max})$ )=Imag( $\varepsilon_m(\omega_{1max})$ ), for chosen dielectric function is fulfilled,  $\omega_{1max}$  is indicated by white dashed lines in figure 2. Volume modes primarily exhibit for frequencies higher than  $\omega_{1max}$ , in the range of lower frequencies Langmuir waves propagate. Second maximum located at frequency  $\omega_{2max}$ , where dispersion curve of the first volume mode, which also owns properties of antisymmetric surface mode [13], intersect with dispersion of the light cone.  $\omega_{2max}$  is indicated by black dashed lines in figure 2.



Figure 2. The angular dependence of the Purcell factor over the frequency, calculated by Eq.(9) for TM polarization, with the dipole oriented perpendicular to layers. The dipole is located in the central dielectric layer  $d_c$ , at the following distance from the left mirror of the system: (a)  $\mu_{point} = \frac{d_c}{2}$  and (b)  $\mu_{point} = \frac{d_c}{60}$ .

We can see that when the dipole is close to the metal-dielectric boundary figure 2(b), in the frequency interval between black and white dashed lines, that corresponds to the hyperbolic regime  $\varepsilon_{\perp}(\omega) \times \varepsilon_{\parallel}(\omega) \leq 0$ , the number of Langmuir modes increases. In the case of anisotropic metal layers it was shown in [12] that the penetration of the electromagnetic field of Langmuir waves into dielectric layers decreases exponentially and predominantly concentrated in metal layers. Therefore in case when the dipole located in the center of dielectric layer only few Langmuir modes can be noticed, in contrast, when the dipole placed closer to the boundary of the metal and dielectric layers more Langmuir modes can be distinguished.



Figure 3. The angular dependence of the Purcell factor over the frequency, calculated by Eq.(10) for TE polarization, with the dipole oriented parallel to layers. The dipole is located in the central dielectric layer  $d_c$ , at the following distance from the left mirror of the system: (a)  $\mu_{point} = \frac{d_c}{2}$  and (b)  $\mu_{point} = \frac{d_c}{60}$ .

When the dipole is parallel to layers: the angular dependence of the Purcell factor for TE polarization, calculated by Eq. 10, is presented in figure 3. The dipole position does not have significant influence on the dispersion properties of TE waves. We can note an enhancement of spontaneous emission for a range of frequencies and angles of incidence related to the allowed band, and inhibition of spontaneous emission for frequencies and angles corresponding to the stop band region.



Figure 4. The angular dependence of the Purcell factor over the frequency, calculated by Eq.(11) for TM polarization, with the dipole oriented parallel to layers. The dipole is located in the central dielectric layer  $d_c$ , at the following distance from the left mirror of the system: (a)  $\mu_{point} = \frac{d_c}{2}$  and (b)  $\mu_{point} = \frac{d_c}{60}$ .

Figure 4 illustrates the Purcell factor calculated by Eq. 11, for TM polarization and parallel orientation of the dipole. We observe similar enhancement of the spontaneous emission in cases when the dipole located in the center (a) and close the edge (b) of the central dielectric layer. In the latter case (b) the number of visible Langmuir modes does not increase as in the case of perpendicular orientation of dipole, since the electromagnetic field of Langmuir waves primarily oscillates in the direction perpendicular to the plane of metal layers.

## 4. Conclusions

In summary, we have calculated the angular dependence of the spontaneous emission of the dipole emitter centered in the periodic metamaterial, designed by alternating metal and dielectric layers. It was shown that the enhancement occurs when the dipole emission is resonant with volume, surface and Langmuir modes of the metamaterial system. We have studied the Purcell effect depending on the position of the dipole source in metamaterial. It was demonstrated that varying the position of dipole mainly affect the interaction with Langmuir modes, which are very important for analysis of metaldielectric structures composed of thin layers. When the dipole approached to one of the mirrors, the Purcell factor begins to grow and reaches the limit exactly on the border of the mirror.

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