Master in Photonics

MASTER THESIS WORK

Optical nanoantenna optimization for local field enhancement at visible wavelengths

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Presented on date 20th of July 2009

Registered at

Escola Tècnica Superior
d'Enginyeria de Telecomunicació de Barcelona

Optical nanoantenna optimization for local field enhancement at visible wavelengths

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Abstract. Dipole nanoantennas are studied by means of numerical calculations, over a broad frequency range (250-600 THz), in order to evaluate the benefits of its integration in NSOM microscopy systems. Operational wavelength, radius and material were systematically varied to study the antenna's resonant length, the field confinement, enhancement and decay. To perform more accurate calculations we implemented an algorithm to include real metal dispersion, at optical wavelengths, in the simulation. The simulations' results suggest that the antenna's performance depends strongly on the material's dielectric properties; even aspects that we would relate only with the antenna geometry like field confinement. By comparing gold and aluminum antennas we found a crossover wavelength for the antenna performance. Below this wavelength aluminum is a more suitable material while for larger wavelengths gold gives better results.

1. Introduction

In everyday life we are accustomed to see radio frequency antennas. These antennas are used to couple electrical signals from a feeding source to free space or vice versa, working in transmission or reception mode respectively. Antennas may be omnidirectionals or directionals. The last ones concentrate the radiation in specific directions of the space when acting as transmitter. Or any type of antenna, when working as receptors, can concentrate the energy in a volume much smaller than the operational half wavelength. These properties are important advantages if we try to avoid a well known problem in optics: the diffraction limit.

1.1. The diffraction limit

Light can not be concentrated in a region smaller than half its wavelength (λ) using a lens system due to the diffraction limit [1]. The diffraction limit imposes a maximum resolution, for a system, which is related to its numerical aperture (NA):

$$r = 0.61\frac{\lambda}{NA} \tag{1}$$

This resolution limit (r) is normally rounded, for common modern objectives with $NA = 1.3$, to $\lambda/2$.

The diffraction limit issue must be overcome if scientists and engineers want to make better lithographic processes, more precise optical microscopes or any other processes involved in nanoptics. If in the macroscopic world at radio frequency it is possible to concentrate the energy in a volume smaller than half wavelength, will it be possible in the nanoscopic world at optical wavelengths? Yes, and it is possible to use the same ideas: antennas. And why could antennas be useful to avoid the diffraction limit? The main reason is because the diffraction limit only applies to the propagating waves, i.e. the far field. Antennas, of any size, radiate in the far-field, though they also couple to the near-field. The near-field or evanescent field does not propagate and rapidly vanishes. So using this evanescent waves we are able to beat the diffraction limit [1].

The first successful experiment beating the diffraction limit dates back to the middle eighties, with two different approaches: sub-wavelength apertures [2, 3] and resonant nanoparticles [4]. Nowadays these two approaches are still the basis of modern near-field scanning optical microscope (NSOM) techniques. The conventional NSOM is based on a sub-wavelength aperture at the end of a glass fiber. Its main problem is that the system's resolution is proportional to the aperture size (a) and system's throughput energy is proportional to a^{-6}. The smaller the aperture, greater resolution, the smaller output power. This is the reason why the aperture is limited in practice to a minimum diameter of about 70nm. As an alternative to the aperture NSOM, exists the "apertureless" NSOM. It consists of a sharp metallic tip, at the end of which the field is locally enhanced. The main problem of the scattering tip is the discrimination between the light used to excite the local field at the tip and the actual local field signal. But the combination of these two ideas lead to maximize the pros and minimize the cons of both. The tip on aperture (TOA) scheme, combining a sharp tip at a subwavelength aperture, was first presented by *Frey et al* [5] who combine high resolution from apertureless NSOM and the background free aperture NSOM.

1.2. Nanoantennas

It has been proven that using nanometric metal structures, it is possible to focus radiation under the diffraction limit [4, 5, 6]. These nanostructures could be understood as nanoantennas in the way that they are used to confine energy in a small region. As with macroscopic antennas, the size, shape and material of the structure define its resonant wavelengths. Or ,the other way around, the operational wavelength determines the rest of parameters. Since these structures have a size of tens or hundreds of nanometers, they will resonate at optical frequencies, i.e. wavelengths from hundreds of nanometers to some microns.

The characteristics of the metal used to construct the nanostructure are critical. At optical frequencies metals does not behave like metals at low frequencies where antenna theory is highly developed.

2. Objectives

In this thesis we are focusing only in a very simple antenna structure: a metal rod made of aluminium or gold with variable length and radius, a dipole. We want to determine which dipole configuration (length, radius and fabrication metal) is the best in terms of field confinement, enhancement and decay for different wavelengths, keeping in mind that these nanoantennas will be used to enhance the performance of NSOM. Since we are simulating two different materials, we should also ask ourselves whether the material plays a crucial role in the performance, which material is better for which wavelength regimes, and why this is the case.

3. Simulation framework

To carry out this work we have used a commercial simulation software: CST Microwave Studio. This software has his own design tools, so specifying a simple structure as a rod is extremely easy. The parameters in our study were radius, wavelength and material. Length is not a variable parameter since we took the length that offers the best field enhancement at the tip of the rod. In order to specify real metals we have created a numerical script to fit the Drude model into the experimental data of dispersion coefficients.

3.1. Software

As we said above, the software used to simulate the metal nanoantennas was the CST Microwave Studio, is provided by the German company of the same name. CST Microwave Studio calculates the field at every time in every point of the meshed structure of the rod and space around it by solving Maxwell's equations. To solve the Maxwell's equations the program uses a numerical finite-element technique called Finite Integration Technique (FIT) [7]. The simulated frequency range goes from 0 Hz to 650 THz, covering from radio frequency and below to the visible light and near UV.

3.2. Nanoantenna structure

The antenna's structure, as described above is similar to a rod. More precisely a tubular shape with a semi-sphere of the same radius of the tube each end. Different radii and material were tested, whereas the antenna length was set to produce a first order resonance. The relation between antenna's length and the radius, material on one side and the radiation's frequency used to illuminate the structure will be discussed in the next section.

As we state in sections 1.1 and 2, our objective is to enhance the performance of TOA-NSOM system. The TOA-NSOM can be modeled as a quarter wave grounded dipole. Antenna theory says that the resonant length of the quarter wave grounded

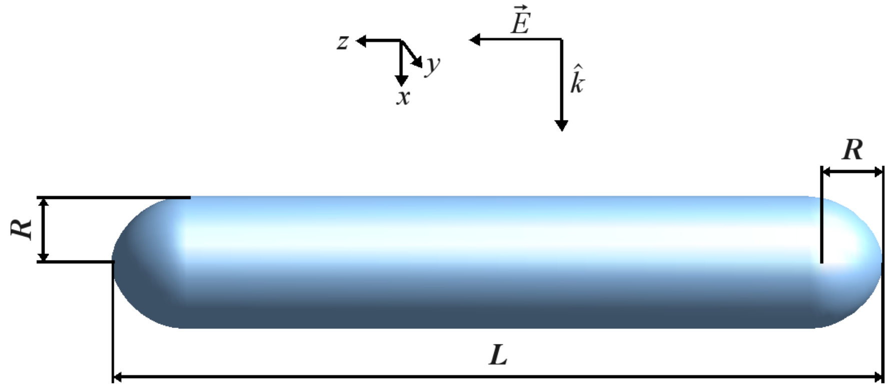

Figure 1. Structure of the nanoantenna: a cylinder of length $L - 2R$ and two semi-spheres, of radius R, at its ends. Thus the nanoantenna's total length is equal to L.

dipole is one half of the free standing dipole. So we can extrapolate our simulation results to the tip used in the TOA-NSOM.

3.3. Metal description

CST offers different possibilities to specify real materials, and more precisely, real metals. Our problem was that metals in the optical range do not act like a perfect conductor or like a metal at low frequency. CST Microwave Studio has some models to describe the metals' behaviour. The model we have chosen is the Drude model.

Drude model was chosen for different reasons. First, because it is a theoretical description of an electrons gas, which behave like metals in almost every frequency range. Second, because of the low number of parameters to adjust in the model, only three. And last because the model fits, more or less, the tendency of the experimental data. To choose the model parameters needed for the CST software we use a numerical routine that fits the experimental dielectric data values at the desired wavelength and approximates the dielectric function around this point.

4. Simulation results

After the simulation of the metallic structures it is time to look at the results. What we get from CST is the electric field at every mesh-point of the rod and its surroundings, with a certain phase. This phase could be used to study how the field evolves in time, but this is not our aim, specially when we are just looking for the field at a certain wavelength, then the field evolution will be harmonic. We studied the electrical field squared because we are interested in the energy confinement, and energy is proportional to $|E|^2$. We focus on the field values at plane yz. It is necessary to say that the wave front travels through the x axis, thus perpendicular to the study plane. It is possible to assume a revolution symmetry of the antenna mode along the axis of the antenna, the z direction, due to the antenna's geometry. This assumption makes possible to extrapolate

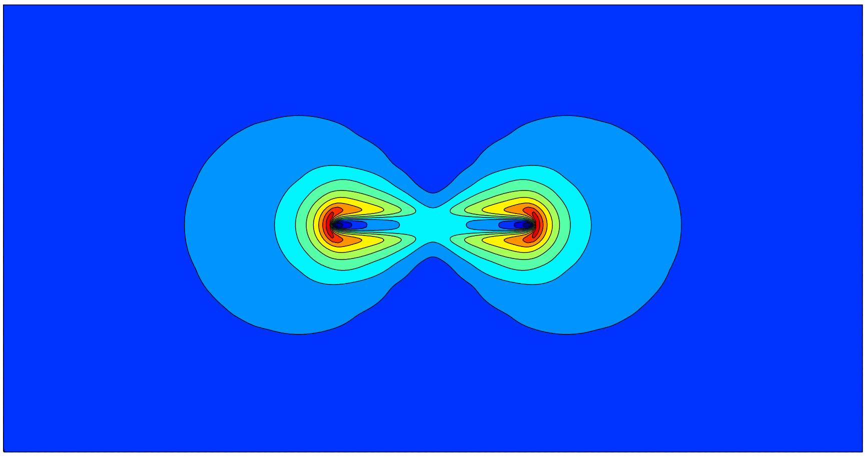

Figure 2. $|E|^2$ on plane yz calculated using CST software. It is possible to see how the field is localized at the end of both tips. Field values are in logarithmic scale.

the results studied in the plane yz to the whole space. In figure 2 the electrical field squared at the plane yz is shown. It is possible to appreciate the field confinement and enhancement at dipole tips.

4.1. Resonant length

First of all, we wonder how the length of resonant antennas change as the operation wave length is changed (Figure 3). The resonant length was determined by varying systematically the antenna length and choosing as L_{res} the one that produces the highest field enhancement at the antenna tip. Simulation results show that, for both materials and both radii, the statement of the macroscopic antenna theory that says that the resonant length of a dipole antenna is $\lambda/2$ is not true in the nanoscopic scale. Here we find an interesting difference between aluminium and gold. The resonant length of the aluminium rods remains constant in terms of wavelengths $L_{\text{res}}(R = 10\text{nm}) \approx 0.22\lambda$ and $L_{\text{res}}(R = 20\text{nm}) \approx 0.3\lambda$. But the resonant length of the gold antenna is reduced as the wavelength is decreased. This phenomenon is strongly related to the dielectric properties of metals. In figures A3 and A4 it can be seen that the values of the dielectric constant for gold are close to zero at high frequency; in that regime the plasmon resonance results in a very short resonance length. In contrast aluminum has a plasma frequency in the UV and behaves as a conductor at all wavelengths considered. The difference between the lengths of antennas made of the same metal but having different radii is quite constant. Also, data shows that the thinner antenna needs to be shorter than the thicker one to operate in resonance.

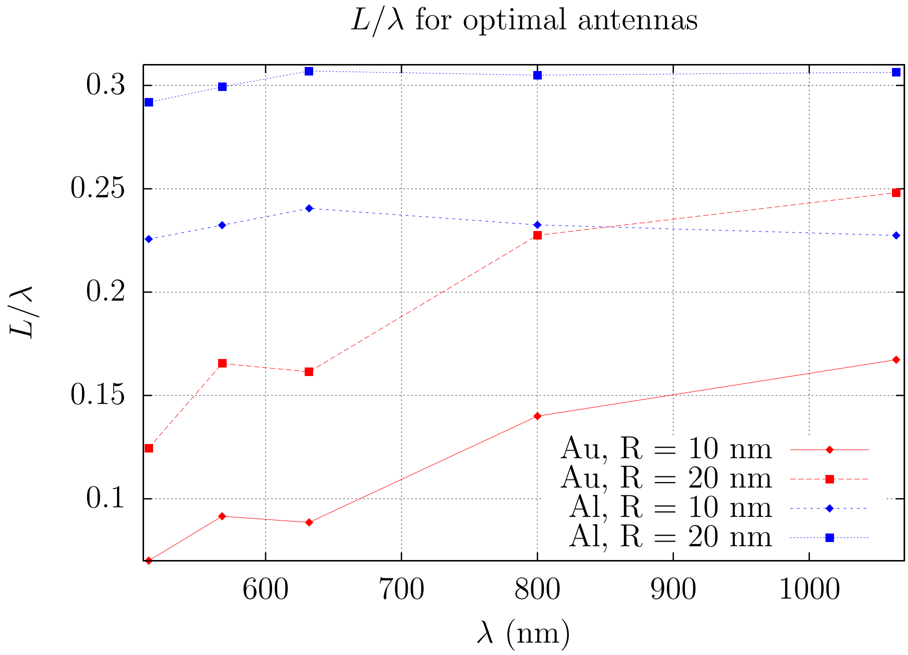

Figure 3. Resonant lengths for different antennas in terms of electrical length.

Our results for gold agree with those calculated by Bryant [8]. For a 20nm radius, results are the same, since resonance length is calculated with the near field, at z=1 nm; and for the radii equal to 10 nm, although Bryant calculated the resonant length through the scattering cross section, our results agree with his.

4.2. Field confinement

The next aspect to analyze is how the field is confined near the tip of the metallic rod and how the area where the field is confined evolves as we get farther away from the tip. This parameters should be very important for anyone who wants to build a NSOM using nanoantennas, since the field confinement fixes the maximum definition of the microscope. In order to quantify the field confinement we define a parameter: the full width half maximum (FWHM). This is a parameter commonly used to describe the width of a "bump" on a curve or function. It is given by the distance between points on the curve at which the function reaches half of its maximum value.

Returning to the possible use of nanoantennas in NSOM, it is important to remember the problem of light confinement in optical systems due to the diffraction limit. The diffraction limit imposes a maximum resolution, or confinement, equal to 0.5λ, as stated in section 1.1.

Now we can define the resolution of a possible NSOM with a nanoantenna as the FWHM. So we are able to compare a NSOM with a nanoantenna to a modern optical microscope. The FHWM has been computed for aluminium and gold rods of two different radii, 10 nm and 20 nm, for every operational wavelength under study.

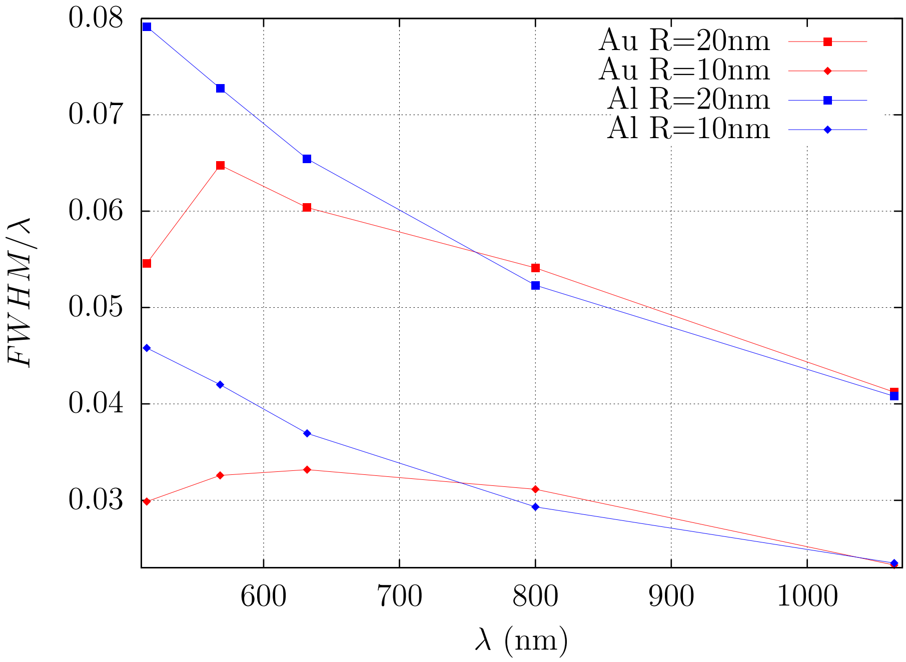

Figure 4. $FWHM/\lambda$, or resolution, at $z = 1$nm away from the tip.

In every case it is possible to appreciate a enhancement of the resolution. At every operational wavelength and at any distance of the tip, ranging from 1 nm to 50 nm, the nanoantenna definition is better than the lensing system.

It is easy to see that for every configuration gold is better than aluminium for shorter wavelengths. But for longer ones, the FWHM is the same on both metals at any distance from the tip. And obviously, the smallest radii has a better field confinement. It is also possible to note that the best field confinement relativ to λ takes place at longer wavelengths, figure 4. But the smallest value of FWHM, in nm, is obtained with gold at 514 nm (figure 5), the shortest wavelength under study.

So we can state, looking at the results, that sharper nanoantennas give higher resolutions. For shorter wavelengths gold is the best option independently of the radius. And for the longer wavelengths the resolution, relatively to the wavelength, is better than the others.

Here we could see an interesting phenomenon also related to the dispersion of gold an aluminium. Aluminium $FWHM$ (in nm) remains constant in all studied wavelengths. The differences in the aluminium resolution are determined only by the antenna radius; whereas gold resolution not only depends on the radius, but also on the wavelength. This could be explained, like the resonant length behaviour, by the materials properties.

Resolution is an important parameter for a NSOM system, but it is not the only one. The other key parameter is the field enhancement. Because a NSOM system with a large resolution but a poor field enhancement, or throughput power, is completely useless. Also, it is interesting to talk about the field decay. All these questions will be discussed in the next section.

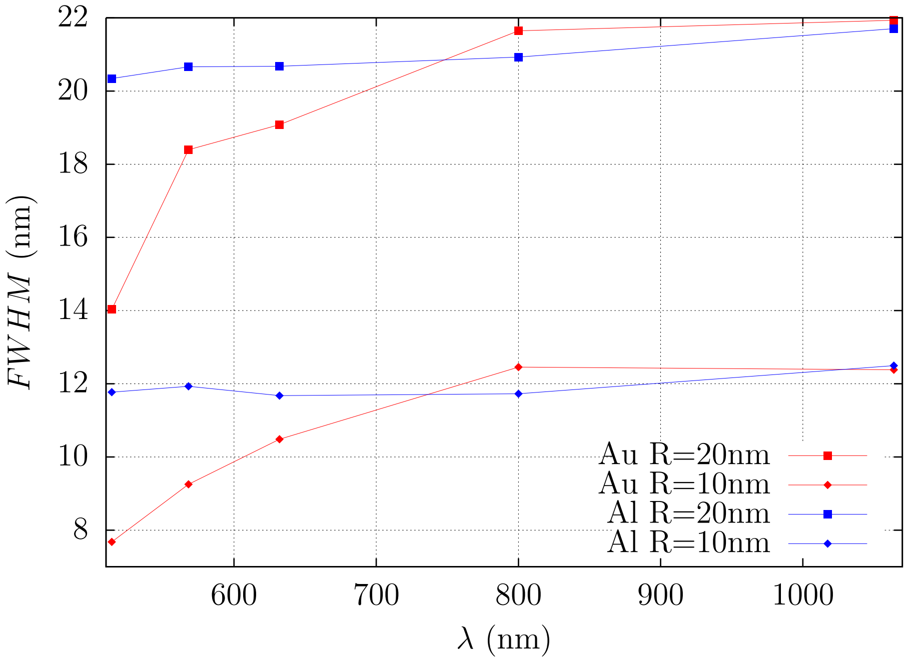

Figure 5. FWHM at $z = 1$nm away from the tip.

4.3. Field enhancement and decay

After analysing the data concerning the field confinement, it is time to look at the field enhancement. Metallic structures can concentrate the field in the confinement region and achieve greater energies. Also, it is important to look carefully at how the field decays along the axial direction of the structure. This is important because it plays an important role determining how close the tip should be approached to the sample under observation, since the main use of the nanoantennas will be as part of a microscope system, the TOA-NSOM.

What we will find will be an evanescent field, so its decay should be something similar to an exponential. But as we will see in a while the exponential decay seems to be different for the different radius structures. In fact this phenomenon is only related with the radii.

Near the tip of the rod ($z < 10$nm) for shorter λ, 514 and 568 nm, the smaller radius aluminium rod has bigger field enhancement. For a intermediate wavelength, 632 nm, it seems that the better option is the thicker gold rod. And for the longer λ, 800 and 1064 nm, the gold rod with smaller radius shows better field enhancement.

When field decay is taken into account a quite strange phenomenon appears. In some cases, near the tip of the antenna, the best field enhancement is performed by the thinnest antennas. But at a given distance, along the z axis, thicker antennas concentrated a higher field. In other words, the field does not decay in the same way

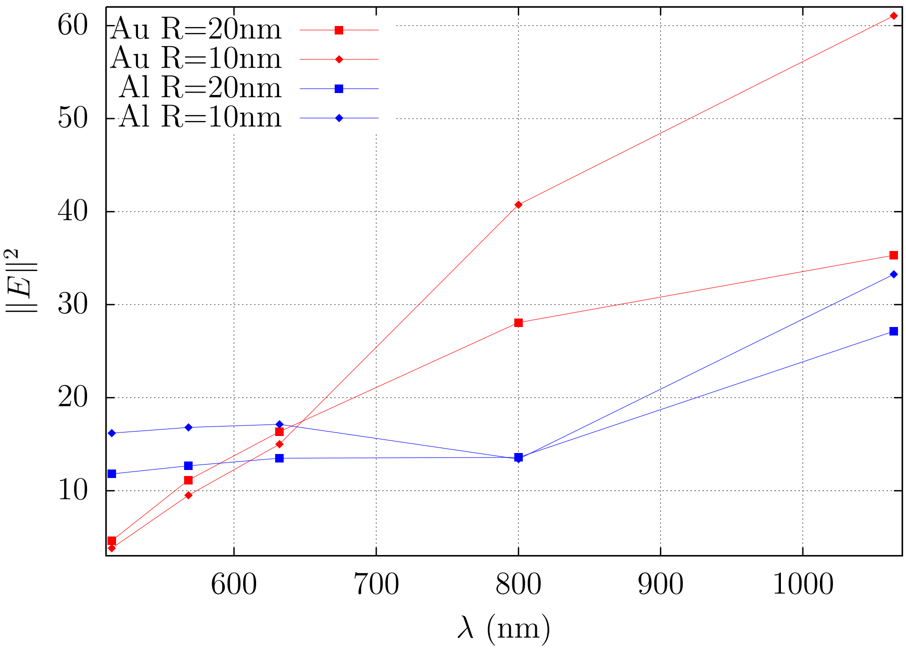

Figure 6. $|E|^2$ at $z = 1$nm away from the tip.

for different radii. The unique explanation for this phenomenon is that field decay depends on antennas' radii. And this can be demonstrated if the field ($|E(z)|^2$) is plotted normalized to its maximum value and taking into account the z distance relative to the radius. At every wavelength, except for 514 nm the field decay is the same for every configuration (radii and material) after this transformation.

Another interesting phenomenon to consider is why the gold rod at high frequencies (514, 568 and 632 nm) produces a slightly better field enhancement with a larger radius (20 nm), see figure 6. This is counter-intuitive, for in the macroscopic world sharper structures generate larger fields at their tips than thicker ones. But at optical wavelengths, as we stated in the two previous sections, gold became fairly transparent to the incoming field. Due to this, the field enhancement for gold under 632 nm is poorer than for aluminium and needs a thicker (and bigger) antenna to scatter a little bit more field. Also we should ask why gold's field enhancement, while aluminium's remains quite constant at every wavelength, grows really fast as the wavelength is increased.

So we can state, looking at the results, that thinner rods usually produce better field enhancement. For shorter wavelengths, thin aluminium antennas generate higher field enhancement. For longer wavelengths, thin gold antennas have the best field enhancement. Thin nanoantenas' field decay is faster than that of thicker ones. This decay seems to be governed by the rod radius. And material's dispersion seems to play a role in the field enhancement: for more transparent material less field enhancement.

4.4. General figure of merit

In order to merge the field confinement and field enhancement parameters in a single one, we calculated a sort of figure of merit (FoM). This FoM is calculated as follows

$$FoM(z) = \frac{|E(z)|^2}{FWHM(z)} \tag{2}$$

This parameter tells us which antenna configuration is the best choice for each situation.

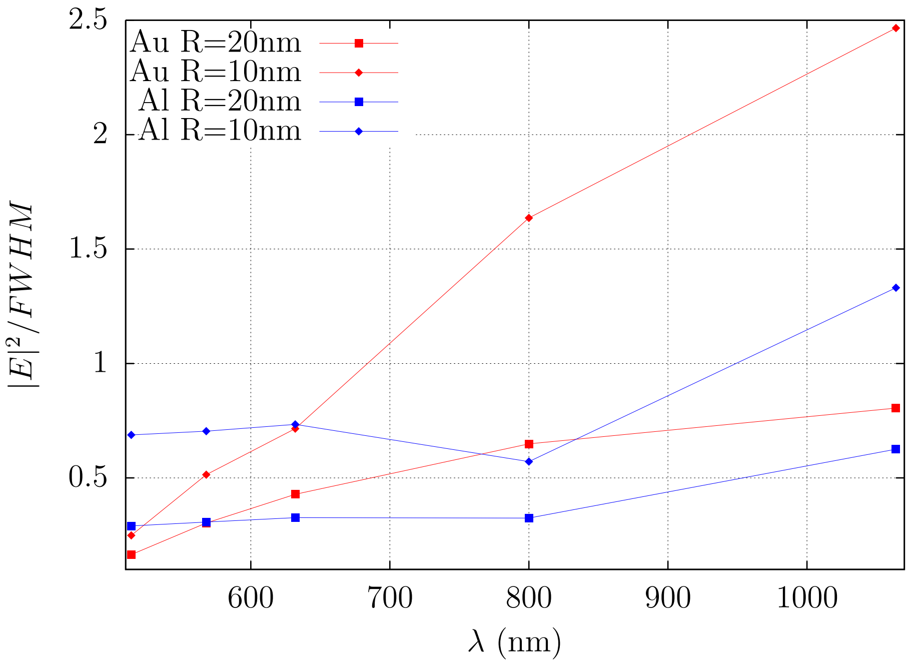

Figure 7. Figure of merit at $z = 1$nm away from the tip.

Now for each wavelength under study we are able to choose the best configuration in agreement to the FoM. For λ equal to 514 and 568 nm aluminium is the best choice for both radii. Near the tip, $R = 10$ nm is the best election. Far from the tip there are not big differences in the performance between the two radii. But, in this case, $R = 20$ nm is slightly better.

At $\lambda = 632$ nm, near the tip, the best choice is $R = 10$ nm but it does not matter whether gold or aluminium is chosen. For $z > 10$ nm the golden nanoantenna with a radius of 20 nm is the best choice. The differences in FoM of the four configurations operating at this wavelength are pretty small. So it is possible to talk about a transition wavelength between aluminium and gold as the best nanoantenna material.

For wavelengths equal to 800 and 1064 nm, the best choice is gold at any distance from the tip. In both cases, thinner antennas have the best FoM near the tip. For $\lambda = 800$ nm and far from the tip ($z > 20$ nm) it is better to switch to the thicker antenna. For $\lambda = 1064$ nm the same happens whenever $z > 30$ nm.

We can see that FoM is strongly determined by the field enhancement. It could be useful to introduce weighting parameters to give more importance to the confinement or to the enhancement. According to the calculated FoMs' values, it is possible to build a table, table 1, with the better configuration for each situation.

Table 1. Resume of the optimal configurations for each wavelength at different distances from the tip.

λ (nm)	Near the tip ($z < z_c$)	Far from the tip ($z > z_c$)	z_c (nm)
514	Al, $R = 10$ nm	Al, $R = 20$ nm	25
568	Al, $R = 10$ nm	Al, $R = 20$ nm	20
632	Al/Au, $R = 10$ nm	Au, $R = 20$ nm	10
800	Au, $R = 10$ nm	Au, $R = 20$ nm	20
1064	Au, $R = 10$ nm	Au, $R = 10/20$ nm	30

5. Conclusions

In our study we have shown that nanoantennas could be used to improve the NSOM performance. At the antenna tips, the field is highly enhanced and confined. The confinement area of the field, for any configuration of the nanoantenna, is much smaller than the diffraction limit. We have confirmed that, for thin antennas, the field is confined in smaller areas than for thick antennas independently of the metal. Also, we have found that field decay, along the axial direction, depends only on the radius of the antenna. Due to this we can state that in order to operate near the antenna tip, we should use a small radius rod, or a thick one if the tip has to be kept away from the sample.

Also, we have determined that a crossover in the material performance exist around 650 nm. Under this wavelength the best performance is achieved by aluminium; whereas gold is more suitable for longer wavelengths. This change in the nanoantenna behaviour is determined by the metal properties. In fact, resonant length, field enhancement and also field confinement are partially determined by the material. And these are the factors that determine the antenna performance. The more close the metal's dispersion relation is to the perfect conductor's, the better the antenna performance will be.

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