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Single-Element Nanoantennas for Ultra-directive Emission

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Abstract. In this report we discuss the possibility of obtaining directional emission through the near-field interference of simultaneously driven electric and magnetic dipole moments in a nanoantenna. Further we discuss which phase relationships are necessary to obtain a high directivity and which geometries are able to meet these requirements. We investigated these geometries with a commercial FDTD - suite and used the recorded electromagnetic fields to model their scattering properties with Mie theory. This enabled us to calculate the spectral dependence of the scattering cross - section of every multipole component up to the octupole for any scatterer.

Keywords: multipole interference, nanoantennas, directivity, mie theory

1. Introduction

With his experiments on oscillating dipoles H. Hertz proved that a dipole could be used as both source and receiver of electromagnetic radiation, and thus set the foundation stone of modern wireless telecommunication. Following Hertz, scientists and engineers designed all kind of antennas for specific purposes. A horn antenna, for example, has a highly directive emission, for a certain direction this leads to a higher interaction efficiency with propagating waves if used as a receiver, or to a higher ratio of signal to feeding current if used as an emitter. Light is electromagnetic radiation like the radio signals we use to transmit information but of a much shorter wavelength. The emission wavelength of an antenna is proportional to its size through its oscillating frequency \( \omega_0 = 1/\sqrt{LC} \), and thus by decreasing the size of an antenna we reduce the wavelength at which it is resonant. To achieve an emission at visible frequencies very small structures, in the order of tens of nanometers, are needed. The race towards the bottom, driven by the need of the semiconductor industry to achieve higher transistor densities, led to advances in lithographic techniques that enable us to produce such structures. Various groups demonstrated directional emission of quantum dots coupled to metallic structures with the size of a few hundred nanometers. Perhaps the most notable example is the nanoscale Yagi-Uda antenna reported by Curto et al. [1]. Since then other geometries have been studied, particularly that unidirectional emission can be achieved using single - element antennas [2] [3] [4]. The principle of operation of these antennas differs from the Yagi-Uda configuration in that instead of off-setting distinct dipolar
elements, these single-element antennas are driven at higher-order resonances which have non negligible multipole contributions, giving a directional emission through self-interference. The multipole components of the fields scattered by an antenna (or any other particle that is similar in size to the wavelength of its illuminating plane wave) can be described by Mie - scattering. The scattering parameters describing the problem can be obtained through a field expansion, or vice - versa if the fields are known. Through FDTD - simulations, the scattering parameters can be retrieved, as demonstrated by Mühlig et al. [5], to characterize the properties of particles for which no analytical solution can be obtained. The general solution close to an arbitrary source can be derived as the field expansion of the spherical harmonics and was numerically implemented by Grahn et al. [6].

In this work we calculated the electromagnetic fields and their properties close to nanoantennas using a commercial FDTD electromagnetic field-solver [7]. The fields were recorded by a spherical monitor consisting of thousands of point monitors. To retrieve the scattering parameters we transformed the recorded Cartesian field components into spherical coordinates. The often neglected radial part of the electromagnetic field was then used to retrieve the total scattered field as shown by Bouwkamp et al. [8].

2. Multipole Expansion of the Scattered Fields

The scattering properties of an arbitrary scatterer in the far field are analysed by expanding the total field on a sphere enclosing all the radiating sources. The fields are represented by Debye potentials and are therefore closely related to the radial components of the electric and magnetic field vectors. The electric and magnetic fields enclosed by the sphere can be represented by imaginary surface currents on the sphere which are equal to the dot products $r \cdot E$ and $r \cdot H$. The fields outside the sphere are derived from these currents and may be represented by a multipole expansion of the spherical harmonics [8]. The electric and magnetic fields are described by:

$$\textbf{H} = \sum_{l,m} [a_E(l, m) h_l^{(1)}(k, r) X_{l,m} - \frac{i}{k} a_M(l, m) \nabla \times h_l^{(1)}(k, r) X_{l,m}]$$

$$\textbf{E} = Z_0 \sum_{l,m} \frac{i}{k} a_E(l, m) \nabla \times h_l^{(1)}(k, r) X_{l,m} + a_M(l, m) h_l^{(1)}(k, r) X_{l,m}$$

where $Z_0$ is the vacuum impedance, $a_E(l, m)$ and $a_M(l, m)$ are the electric and magnetic scattering coefficients, $h_l^{(1)}(l, m)$ is the spherical Hankel function of the first kind and $X_{l,m}$ the vector spherical harmonic.

The field at the surface of such a sphere can be calculated using modern field solvers. In our case we used 1225 point-monitors surrounding the scatterer, forming a sphere with a diameter of 12 µm, this was necessary as our FDTD field solver could not provide spherical field monitors. The Cartesian field vectors were afterwards transformed with a rotation matrix to obtain the field in spherical coordinates. If the field inside the sphere is known, the expansion can be used inversely to analyse the scattering properties of the enclosed
scatterer by obtaining the scattering coefficients as shown by Grahn et al. [6]. The multipole coefficients are represented by equations 3 and 4 for the electric and magnetic multipole components, respectively.

$$a_E(l, m) = \frac{(-i)^l+1kr}{\hat{h}_l^{(1)}(kr)E_0[\pi(2l + 1)(l + 1)]^{1/2}} \int_0^\pi \int_0^\pi Y_{l,m}^*(\theta, \phi) \hat{r} \cdot \hat{E_s}(r) \sin \theta \, d\theta \, d\phi$$

$$a_M(l, m) = \frac{(-i)^lZ_0kr}{\hat{h}_l^{(1)}(kr)E_0[\pi(2l + 1)(l + 1)]^{1/2}} \int_0^\pi \int_0^\pi Y_{l,m}^*(\theta, \phi) \hat{r} \cdot \hat{H_s}(r) \sin \theta \, d\theta \, d\phi$$

$r$ is the radius of the imaginary spherical surface where the fields are recorded, $k$ is the wave vector in the dielectric medium surrounding the scatterer, $\hat{E_s}$ and $\hat{H_s}$ are the electromagnetic fields at the radius $r$ from the origin, $Y_{l,m}^*$ is the complex conjugate of the scalar spherical harmonics, $\hat{r}$ is the radial unit vector, and $E_0$ is the magnitude of the incident field equal to unity in our simulations.

Following Grahn et al. the Cartesian multipole components up to the magnetic quadrupole mode are expressed by the following equations. In our simulations we recorded the modes up to the magnetic octupole mode.

$$p = \begin{pmatrix} p_x \\ p_y \\ p_z \end{pmatrix} = C_1 \begin{pmatrix} a_E(1, -1) - a_E(1, 1) \\ -i(a_E(1, 1) + a_E(1, -1)) \\ \sqrt{2}a_E(1, 0) \end{pmatrix}$$

$$m = \begin{pmatrix} m_x \\ m_y \\ m_z \end{pmatrix} = cC_1 \begin{pmatrix} a_M(1, -1) - a_M(1, 1) \\ -i(a_M(1, 1) + a_M(1, -1)) \\ \sqrt{2}a_M(1, 0) \end{pmatrix}$$

$$Q = C_2 \begin{pmatrix} -\frac{\sqrt{3}}{3}a_E(2, 0) \\ -i(a_E(2, -2) - a_E(2, 2)) \\ (a_E(2, -1) - a_E(2, 1)) \end{pmatrix} - \begin{pmatrix} -i(a_E(2, -1) + a_E(2, 1)) \\ \frac{2\sqrt{3}}{9}a_E(2, 0) \end{pmatrix}$$

$$MQ = cC_2 \begin{pmatrix} -\frac{5\sqrt{3}}{3}a_M(2, 0) \\ -i(a_M(2, -2) - a_M(2, 2)) \\ (a_M(2, -1) - a_M(2, 1)) \end{pmatrix} - \begin{pmatrix} -i(a_M(2, -1) + a_M(2, 1)) \\ \frac{2\sqrt{3}}{9}a_M(2, 0) \end{pmatrix}$$

With $C_1 = -3\pi\varepsilon E_0/(ik^3)$ and $C_2 = -25\pi\varepsilon E_0/(3k^4)$, where $\varepsilon$ is electric permittivity, $k$ the wave vector, $c$ the speed of light in the medium surrounding the scatterer and $E_0$ the magnitude of the field. The diagonal quadrupole components are derived from the analytical solution for a symmetric scattering problem. For a $z$ - symmetric scattering problem $Q_{zz} = -2Q_{xx} = -2Q_{yy}$ according to Landau - Lifshitz [9]. The power radiated by each multipole component is given by equation 9 and the radiation pattern for each multipole can be found in the literature[10].

$$P(l, m) = \frac{Z_0}{2k^2} \sum_{l=1}^{\infty} \sum_{m=-l}^{l} |a(l, m)|^2$$
3. Split Ring Resonators

Pendry et al. suggested in 1998 that metal split-ring resonators (SRRs) may have strong electric and magnetic responses similar to an LC circuit, with the gap forming a capacitor and the loop a coil [11]. These resonances, if a SRR is used as an optical antenna and coupled to a local-source such as a quantum dot, can be used to create directional emitters of sub-diffraction-limited size as demonstrated by Hancu et al. [3]. They showed that the interference between an electric dipole and an electric quadrupole moment at one such resonance can be used to create either forward or backward scattering with a U-shaped SRR. In principle it would be favourable to use low-order modes that provide stronger electric and magnetic dipole responses, as the provide higher scattering efficiency and stronger field enhancement. Furthermore, directional scattering due to the interference of electric and magnetic dipole moments are predicted by Mie theory for a perfect conducting sphere. We optimized a SRR to have a similar strength for the electric and magnetic dipole at the first order (λ/2 resonance (Fig. 2 a)). 2b Shows that, even though the cross-section of the electric and magnetic dipole moments are of similar magnitudes, their emission pattern is non-directional. This is due to the importance of phase between these two main contributions. The maximum directivity is defined by formula 10 and is equal to $D \approx 3.63$ for the simulated SRR which is approximately by a factor two better than that of a single dipole ($D = 1.54$) or that of a linear half wave antenna ($D = 1.64$) [12].

$$D(\theta, \phi) = \frac{\langle dP/d\Omega \rangle}{\langle P \rangle / 4\pi}$$

(10)

Where the gain $D(\theta, \phi)$ is defined as the quotient of the angular power distribution of the scatterer $\langle dP/d\Omega \rangle$ and the average power of the ideal spherical emitter $\langle P \rangle$. 

\begin{figure}
\centering
\includegraphics{figure1.png}
\caption{a) An illustration of a SRR driven by a quantum dot. The light radiated by the quantum dot couples to the structure and induces an oscillating electric current that creates a magnetic field normal to the SRR plane. b) The development of the electric and magnetic field with respect to the phase of the driving field (red) are illustrated by the charges for the electric and the arrows for the magnetic field.}
\end{figure}
Ultra Directive Dipole Interference

Figure 2. The scattering properties of an Al-SRR. The structure is a SRR, as shown in Fig. 1, with an inner radius, $r_1$, of 80 nm, an outer radius, $r_2$, of 120 nm, a height, $h$, of 50 nm, and a gap size, $d$, of 40 nm. The structure is excited by a dipole source placed at the center of the gap and polarized along the gap axis. a) The calculated scattering cross-section over a broadband spectrum for each multipole component up to the octupole. b) The far-field projection at the resonance wavelength, 1886 nm, of the half-space below the SRR plane (that is equivalent to the upper, as the structure is surrounded by vacuum). c) Geometry of the SRR, and orientation of its coupled dipole source.

Fig. 3a shows the pattern of two parallel electric dipoles separated by a distance of $\lambda/4$ normal to the dipole axes and radiating $\pi/2$ out of phase like in the Yagi-Uda configuration.

Further simulations of simple dipoles show highly-directed emission patterns may be obtained as well with perpendicular electric and magnetic dipoles (Fig. 3b). As the fields in the near-field region are quasi-static they can be derived from simple models, where the electric dipole is represented by two separated charges and the magnetic dipole by a current loop. Due to geometric reasons, their respective fields radiate in phase in one direction and $\pi$ out of phase in the opposite, meaning that there is constructive and destructive interference in opposite directions that can be used.

Figure 3. Demonstration of directivity through dipole interference. a) Pattern of two electric dipoles radiating with a phase difference of $\pi/2$ and displaced by $\lambda/4$ b) Pattern of a crossed electric ($p_x$) and magnetic ($m_z$) dipole radiating in phase. The top row shows their far-field radiation patterns and the bottom the phase difference between their electric fields along the $y$-axis. Note that for both dipole arrangements a high backward directivity is observed as the fields are in phase in the backward direction and $\pi$ out of phase in forward.
For a SRR the crossed transverse electric (TE) and transverse magnetic (TM) fields are expected to be an additional $\pi/2$ out of phase if the SRR behaves like a classic LC-circuit. The phase change of $\pi/2$ of the TM-field with respect to the TE-field leads to an emission, that is, if at maximal phasematch, in phase in the direction of one axis and $\pi$ out of phase for the axis normal to it (4 a). A change of distance between the dipoles inverts the axis (4 b). Consequently a change of the distance between the dipoles cannot change the phase relation in one plane, so unlike to the Yagi - Uda configuration represented by Fig. 3a a symmetric pattern is observed and directivity cannot be obtained by changing the distance between the dipoles. Thus a different geometry must be utilized if a directional pattern from interfering electric and magnetic dipoles is to be achieved.

4. Dielectric Sphere

Like the previously-analysed SRR, spherical dielectric particles are also known to support strong magnetic dipole modes. For an ideal spherical conductor, Mie theory can be used to find a solution where only few terms are needed in the expansion. If a plane wave impinges a perfectly-conducting sphere the field generates a surface current. This current generates a TM - field that seems to originate from the spheres center, forming a magnetic dipole which is crossed with the emitted electric dipole field. Both dipoles oscillate in phase so the condition illustrated in 3b is met. The modes are described by Mie theory through Debye potentials as the field is distorted by charges forming on the particle surface. The solutions inside the sphere are Bessel functions and outside Hankel functions of the first and second kind, so the field decays towards infinity [13] [14].

Figure 4. A demonstration of the impossibility of obtaining a directional emission between a perpendicular electric ($p_x$) and magnetic ($m_z$) dipoles when they are $\pi/2$ out of phase. a) and b) correspond to $\lambda/4$ and $-\lambda/4$ displacements between the dipoles along the axis perpendicular to their orientations (y-axis). The top row shows their far-field radiation patterns and the bottom the phase difference between their electric fields along the y-axis, with red being $p_x$ and orange $m_z$. Note that for a) the phase difference in opposite directions are 0 and $2\pi$ whereas in b) it is $\pi$ for both, in contrast with Fig. 3 b (bottom).
B. R. Johnson developed a theory describing these resonances with a model inspired by quantum mechanics. The particle forms an energy well with certain quantized states. The potential of the well is connected to the shape, size and complex refractive index of the particle. The field enters the particle by tunnelling through the potential wall. In the well a self-sustaining standing wave forms a whispering gallery mode, such a mode is similar to a circular current and leads to an orthogonal magnetic field (See Fig. 5, adapted from [15]). Figure 6 shows the scattering cross-section for the different modes in a TiO$_2$ particle source at a distance of $d = 15$ nm.

Strong directivity occurs when the magnetic dipole and quadrupole term are of similar magnitude forming a transverse magnetic field similar to directional, higher order nanoantennas. It is unclear if the scattering occurs purely due to the magnetic multipole terms as the electric quadrupole and the magnetic octupole are also non-negligible in this part of

**Figure 5.** An illustration of a dielectric sphere with its whispering gallery modes. a) the red loops correspond to the electromagnetic field of the light trapped in the cavity mode, and the green lines are the resulting magnetic fields. b) The wave-function of the field inside the cavity-model used by B. R. Johnson, with the top and bottom showing forbidden states not leading to resonances, and a resonance state in the middle [15].

**Figure 6.** The scattering properties of a TiO$_2$ sphere with a radius of 200 nm illuminated by a local electric dipole source in the plane tangential to the sphere’s surface and 15 nm away from it. a) The scattering cross-section of the different multipole components over a broad spectrum from 400 – 1200 nm. b) the far-field projection at the wavelength showing the maximum directivity ($\lambda = 920$ nm). c) Geometry of the structure and orientation of its coupled dipole-source.
the spectrum. TiO<sub>2</sub> was used as it combine a low absorption in the visible spectrum and a high refractive index, which enables structures way smaller than the illuminating wavelength, so geometrical effects can be reduced.

Small metal nanoparticles on the other hand support strong electric-dipole modes due to charge oscillations. [16]. A combination of both seems to be promising way to obtain directional near field scatterer through interference of the electric and magnetic dipole. Recently Liu et al. proved theoretically that such particles show strong forward scattering if illuminated by a plane wave [17]. We simulated different core shell nanoparticles configurations and Fig. 7 illustrates the scattering behaviour of a dielectric core \( r_1 = 200 \) nm which is coated with aluminium \( r_2 = 205 \) nm when illuminated by a electric dipole source at an equatorial distance of \( d = 15 \) nm.

**Figure 7.** The scattering properties of a TiO<sub>2</sub> sphere with radius, 200 nm and a 5 nm aluminium coating illuminated by a local electric dipole source in the plane tangential to the sphere’s surface and 15 nm away from it. a) The scattering cross-section of the different multipole components over a broad spectrum. b) The far-field projection for a wavelength of 1124 nm where the electric and magnetic dipole moments have the same cross-section. c) Geometry of the structure and orientation of its coupled dipole source.

Notice that the coated sphere behaves generally similarly to metal nanoparticles at long wavelengths towards the IR region a strong electric dipole oscillation can be observed and the directivity is poor. This can be explained by the low skin depth of aluminium at long wavelengths. If we stay in the model of Johnson the aluminium coating increases the potential barrier and reduces the field tunnelling into the particle. Consequently the circular field inside the sphere is very weak and the amplitude of the magnetic dipole mode is much lower than the electric. Towards shorter wavelengths the field can tunnel into the particle and the directivity improves. A maximum directivity of \( D \approx 6.65 \) can be observed at a wavelength of 1124 nm where the electric and magnetic dipoles are of similar strength. The not totally suppressed forward scattering hints towards an imperfect phase matching, though much improved compared to the previously-studied SRR shown in Fig. 2b. For the inverted particle with a metal core and a dielectric shell the multipole terms can be gradually changed to some degree by tuning the diameter of the metal core, as illustrated in Fig. 8 which shows...
the total scattering cross-section $C_{\text{Scat}}$ for a Al/TiO$_2$ core-shell nanoparticle with different core diameters.

The core-shell nanoparticle with a core diameter of 180 nm shows both high directivity and a high scattering cross-section. Fig. 9 shows the multipole moments up to the octupole terms between 400 and 1200 nm. Between 950 and 1150 nm a high backward directivity is observed with the highest directivity of $D \approx 9.64$ occurring around 1087 nm where the amplitudes of the magnetic and the electric dipole moments intersect. Surprisingly, below 950 nm the directivity strongly decreases even though the electric and magnetic dipoles are of similar strength. This behaviour is likely due to interference with the magnetic quadrupole term, which cannot be considered negligible for wavelengths shorter than 950 nm.
5. Conclusion

In this thesis we implemented a method to analyse arbitrary structures through Mie theory. We used this technique to study the interference behaviour of different nanoantenna structures. Further we discussed that near-field interference of crossed electric and magnetic dipoles can lead to a highly directional emission pattern, and that similar amplitudes and a certain phase relation is required. We found that metal/dielectric core-shell nanoparticles are a promising candidate to obtain a highly directional scattering from an electric dipole source with a pattern similar to that of an ideal conductor.

6. References