Supplementary Material

Controllable Directive Radiation from Dipole Emitter Coupled to Dielectric Nanowire Antenna with Substrate-Mediated Tunability

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The purpose of this document is to outline the semi-analytical formulation and derivation of the closed-form expressions for the field contributions. In the first section, we obtain the field contribution to the scattering. In the second section, closed-form expressions are obtained for field contributions using asymptotic approximation in farfield. Finally, we validate our developed semi-analytical framework by comparing the results against full-wave finite-difference time-domain (FDTD) simulations.

1. **Dipolar Scattering from a Nanowire on Top of a Layered Substrate**

The geometry of the structure under consideration is shown in Fig. S1. It is made of a cylindrical nanowire of radius located above a layered substrate, excited by a near-by point source. In the present work is chosen parallel to the wire axis (****). The formulation can be extended for transverse magnetic polarization in a similar way. The Cartesian coordinate system , the associated cylindrical **** and spherical **** coordinate systems are introduced, such that the z- axis is parallel to the nanowire axis and the origin coincides with the center of the nanowire while coordinates of the dipole source is ****. A quantum dot emitter is modelled as a dipole placed at its phase center. The separation distance between the nanowire center (origin) and the air-substrate interface is denoted by ****. In the case that the nanowire is seated on top of the substrate ****.



Fig. S1. (a) The 3D view of the problem geometry under study. (b) The cross section of the problem geometry.

In the following, we aim at obtaining analytical expressions for the fundamental field components of **** and ****. The rest of the field components can then be obtained through Maxwell equations. The time dependence of ****, with **** being the angular frequency, is assumed and suppressed.

In the case of a dipole source above a substrate the total field can be expressed as the sum of the incident spherical wave **** and reflection of the incident spherical wave by the substrate ****. Four further terms are produced by the addition of the nanowire namely the co- and cross-polarized scattered fields (**** and ****), and the co- and cross-polarized scattered-reflected fields (**** and ****):

 (1)

 (2)

The scattered fields can be expressed using a multipole expansion with unknown coefficients. The scattered-reflected fields characterize the multiple scattering effects between the nanowire and the substrate which can be obtained using the plane wave spectrum of cylindrical waves through a substrate reflection matrix whose elements are given by Weyl-type integrals [S1]. The unknown coefficients in the multiple expansion can be then obtained by imposing the boundary conditions on the surface of the nanowire.

The incident field due to the dipole source can be expressed as:

 (3)

where **** is the wave number in free-space. Using the Weyl identity and the plane-wave spectrum of the incident field, the reflected field from the substrate due to this incidence can be obtained using angular spectrum of the reflection coefficient as:

**** (4)

where **** is the reflection coefficient of the layered substrate corresponding to the TE polarization, ****, and ****. A scattering matrix-based approach can be used to calculate the reflection coefficient of layered substrates composed of 2D sheets and bulk materials [S2].

Now, in order to obtain the scattered field from the nanowire due to these field contributions, we need to expand them in terms of regular cylindrical harmonics in the local coordinates of the nanowire ****. After that, the scattering from nanowire can be expressed in terms of cylindrical harmonics ****, where the unknown coefficients can be related to the coefficients of the regular harmonics through a matrix formulation enforcing the boundary conditions. It is noticed that **** and **** denote the m-th order cylindrical Bessel function and Hankel function of the first kind, respectively.

Using the Sommerfeld identity, the incident field can be expressed as a spectrum of cylindrical waves:

**** (5)

Using the Graf’s addition theorem [S3], we will obtain the incident field in terms of regular cylindrical harmonics as:

**** (6)

where ****. Expressing the reflected field (4) in terms of regular cylindrical harmonics needs considerably more effort. In order to write (4) in cylindrical coordinates, we let ****, ****, **** and ****. Then, (4) becomes:

**** (7)

Expanding **** and making use of the integral identity for Bessel function [S4],

(8)

We obtain:

(9)

Applying the Graf’s addition theorem [S3], we will arrive at the reflected field in terms of regular cylindrical harmonics as:

(10)

Now, having expressed the incident and reflected fields in terms of the regular harmonics, we can write the co- and cross- polarized scattered fields from nanowire as the sum of primary and secondary scattered fields due to the incident and reflected fields:



(11)



(12)

In the above equations, **** and **** are the coefficients enforcing the boundary conditions on the nanowire surface which can be obtained through a matrix formulation [S1, S5]. The matrix encapsulating the boundary conditions is a 2 by 2 block matrix, defined as:

**** (13)

This matrix relates the coefficients of the regular harmonics to those of the co-polarized and cross-polarized scattered harmonics for a nanowire placed on the layered substrate. The blocks are labelled such that  relates the coefficients of the regular harmonics corresponding to **** to those of the scattered harmonics corresponding to ****. **** and **** are the generalized transition matrix and substrate reflection matrix, respectively defined as:

**** (14)

**** (15)

where:

**** (16)

**** (17)

**** (18)

**** (19)

**** (20)

where **** is the Kronecker’s delta function, **** is the reflection coefficient of the layered substrate corresponding to TE/TM polarizations, ****, **** and:

**** (21)

In the case studied here where the incident and reflected fields are TE-polarized, so we have **** and ****.

Finally, reflected-scattered field contributions can be obtained using the reflection matrix of the substrate as [S1, S6]:

**** (22)

Equation (22) is corresponding to the co-polarized reflected-scattered field. The cross-polarized component can be obtained similarly by replacing ****, **** and **** by ****, **** and ****, respectively.

1. **Asymptotic Approximation of the Field Contributions**

Having obtained all the field expressions, the remaining challenge is to evaluate the highly oscillating and slowly-convergent integrals. Numerical integration schemes are very time-consuming and inefficient. Furthermore, they cannot resolve the far field response accurately. As such, we use the stationary phase method for obtaining asymptotic approximation of the field contributions in the far field [S3, S4]. The method gives closed form expressions for the integrals which is extremely efficient and advantageous for quantification of the performance characteristics in far field. The results are highly accurate to the leading-order and higher order terms can be added if necessary. This approach is very useful for the fast design and optimization in antenna applications [S7-S10].

We consider integrals of type  where  is a large parameter. In the case that the integrand becomes highly oscillating for large , the stationary phase point method can be used to obtain a closed-form approximate formula for the solution of the integral. We rewrite the integral in the form of  such that  is the highly oscillating part which can be integrated analytically (i.e.  has a closed-form) and  is the slowly-varying part. If  when , then by virtue of the stationary phase method argument, contribution to the integral  will come from the point where the phase of the exponential function is stationary (i.e. ) [1, 2]. Then, the asymptotic approximation of the integral is:

 (23)

Before, starting the derivation of the asymptotic expressions for the field contributions, we recall the Sommerfeld and Weyl identities which are used in the approximations [S11]:

 (24)

 (25)

Approximation of the reflected field (4), requires evaluation of the following integral:

 (26)

when *x*, *y*, or *z* are large, the integrand becomes highly oscillating function of  and  because of the exponential term which makes the numerical integration a tedious task. The stationary phase point of the highly oscillating part in the two-dimensional space can be obtained by solving:

 (27)

which gives:

 (28)

where . Having the Weyl identity (25) in mind and using the stationary phase point concept, we rewrite the integral as:

 (29)

Using Weyl identity gives us:

 (30)

Now, we can obtain the closed form leading order approximation for the reflected field as:

 (31)

Next, we consider evaluation of the integrals in the scattered field contribution which have the form of  where  is a slowly varying function of . Such integrals are highly oscillating when  or  tends to infinity according to the large-argument approximation of Hankel function:

 (32)

Having the Sommerfeld identity in mind, we rewrite the integral in the following form:

 (33)

Using (32), the stationary phase point of the oscillating part is obtained by solving:

 (34)

which gives

 (35)

Using the Sommerfeld identity and the stationary phase point scheme, we obtain:

 (36)

which using the large argument approximation of Hankel function (32), can be simplified further to:

 (37)

Using this integration procedure, we will arrive at the following closed form leading order approximation for the scattered field contribution:

 (38)

Let us now consider evaluation of the integrals in the scattered-reflected field contribution which have the general form of . Such integrals are highly oscillating when  or  tends to infinity. However, using the large argument approximation for the Bessel function, we notice that the integrand does not have a well-defined stationary phase point. As such, we use the identity for Bessel functions in terms of Hankel functions [S12]:

 (39)

Replacing this in the field expression, we can evaluate the integrals similar to the integrals in the scattered field contribution. This results into:

(40)

The integrals in the cross-polarized field contributions have the similar form and can be evaluated with the above-mentioned procedures. Once the closed form approximations for  and  are obtained, the derivation of the rest of the field components will be straightforward by application of Maxwell’s equations.

It should be remarked that the higher order terms can be added to the leading order approximations using steepest descent method [S3]. The semi-analytical framework developed in this work can be readily extended for interaction of dipolar sources with gratings of nanowire above layered substrates by taking into account the coupling of multiple scatterers through translation of cylindrical harmonics.

1. **Validation against Full-wave FDTD Results**

In this section, we provide representative results of each design to verify our semi-analytical results and the developed framework. It should be mentioned that the results of the proposed method were obtained by a MATLAB developed code with each simulation taking less than a minute to complete. The maximum number of cylindrical harmonics used for the truncation of the multipole expansions was  which ensures the convergence of the results for the subwavelength wire antennas. The FDTD simulations were carried out using a 3D FDTD in-house developed solver by considering only a few cells along the nanowire axis and touching all the walls into perfectly matched layers. A 2D FDTD is not applicable because of the 3D geometry of the point source. Despite the small size of the computational domain along the nanowire axis, FDTD simulations turn out to be way more time consuming (several minutes) compared to the semi-analytical solutions (a few seconds) because of the fine meshing required for resolving the curvature of subwavelength wire antennas as well as deeply subwavelength features of the active layers in the substrate such as the charge accumulation layer of ITO. Moreover, FDTD requires costly post-processing for transformation of near-field to far-field and obtaining the radiation pattern. The extreme efficiency of the proposed method is best appreciated in the design and optimization of the structures for antenna applications. The geometrical configurations considered in this work have several critical parameters affecting the directionality, gain and the steering range which makes it very challenging to use brute-force methods for the design and optimization.

Figures S2 (a)-(c) compare the results of the proposed method with those of the FDTD for a representative case of each design. The size of FDTD computational domain and the cell size used for discretization corresponding to each case are shown in the figures. The computational domains are chosen sufficiently large along x and y directions for an accurate nearfield to farfield transformation by forward propagating the fields on the top aperture. A typical illustration of the computational domain can be seen in Fig. S2(d) corresponding to the design in Fig. S2(a) where the red dashed lines show the boundaries of perfectly matched layers.

 A great agreement is observed between all the results which verifies the validity of our method. The discrepancies are mainly attributed to the numerical errors inherent in FDTD while semi-analytical solution should give correct results. Additionally, the FDTD method uses an orthogonal and staggered grid for the Yee lattice which leads to numerical inaccuracies for the curved structures [76] due to the shift in the locations at which the field components are evaluated. The agreement between the results are expected to be further improved by using a finer mesh for FDTD discretization and enlarging the computational domain for the transformation to far-field.



Fig. S2. Comparison of the results of the proposed semi-analytical method with those of FDTD for (a) representative case of the first design where , (b) representative case of the second design where  and (c) representative case of the third design where . The size of FDTD computational grid (Tx, Ty, Tz) and cell size used for discretization (Δx, Δx, Δz) corresponding to each case are shown. (d) The typical computational domain for FDTD calculations corresponding to the design in (a) where red dashed lines denote the boundaries of perfectly matched layers and the dipole source is denoted by an arrow along the polarization direction.

**Supplemental References**

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