A More Realistic Coupled Dipole Approximation Model for Plasmonic Waveguides

Ergun Simsek

Department of Electrical & Electronics Engineering
Bahcesehir University, Istanbul, TURKEY
ergun.simsek@bahcesehir.edu.tr

Abstract— **Well-known coupled dipole approximation method is extended to multilayered media to obtain a more realistic model for plasmonic waveguides. The key component of the developed method is the layered medium Green's functions. Theoretically calculated resonance frequencies show a very good agreement with the experimental results found in the literature.**

Keywords-plasmonic waveguides; dispersion; propagation length; layered medium.

I. INTRODUCTION

Surface plasmon resonance modes of periodically placed metal nanoparticle chains and arrays, which are the main element of plasmonic waveguides, have been studied extensively in last two decades. Experimentalists have used transmission and/or reflection spectroscopy in order to obtain dispersion relations of the surface plasmons, whereas theoreticians have developed novel models both in time and frequency domains. Since most of the frequency domain models, developed based on the coupled dipole approximation (CDA), assume a homogeneous background, they are not sufficient and robust to design an optical waveguide for real world applications.

We can summarize the four strategies -applied so far- to validate experimentally obtained dispersion curves/resonance frequencies with a theoretical/numerical model as follows:

(i) *Full Wave Solvers:* One can solve Maxwell Equations in 3D space and apply appropriate boundary conditions to simulate the wave propagation through MNP chain. Such solution is an exact solution (100 percent robust) but might require very long computation time [5-7, 9].

(ii) *CDA with Image Theory:* Koenderink *et al* already applied this solution to calculate the resonance frequencies of MNP chains fabricated on a glass slide [6]. The drawback is the formulation is only valid for the two-layer case (e.g. air-glass).

(iii) *CDA with Effective Refractive Index Approximation (ERIA):* In [7], researchers approximate the whole inhomogeneous background with a single homogeneous medium whose refractive index depends on each layer's thickness and refractive indices. Even though this simple method can estimate resonance modes quite accurately, it still cannot explain the effect of an interface on dispersion modes.

(iv) *Semi-Analytical CDA:* In [9], researchers use a full wave solver to calculate the polarizability of a single MNP first, and then use this result for coupled dipole approximation. This is another very reliable method but requires a full wave solver.

In this work, we extend the CDA to multilayered media by implementing layered medium Green's functions (LMGFs). LMGFs are used not only to calculate the electric field created by the oscillating point dipoles, which are MNPs, but also to modify the polarizability of MNP embedded in multilayered media, appropriately. The formulation is not limited to any fixed number of layers, unlike [10], and does not require an external full wave solver. This fully analytical method includes the effects of retardation, radiative damping and dynamic depolarization due to the finite size of NPs. Theoretically calculated resonance frequencies show a very good agreement with the experimental results found in the literature. Theoretical results suggest that surface plasmon propagation lengths of 1μm are possible using silver or gold nanoparticles embedded in a multilayered medium.

II. LAYERED MEDIUM COUPLED DIPOLE APPROXIMATION

Assume there is a finite chain of equally spaced metal NPs along the **x**-axis in a multilayered medium; M is the number of NPs and d is the inter-particle spacing. Again assume NPs can be represented as oscillating dipoles ($\mathbf{p}_j$, j=1, 2, ..., M) and ω is the oscillating frequency in the absence of an applied field. The induced dipole moment on particle-n because of field generated by dipole-m can be calculated as

$$\mathbf{p}_n = \overline{\overline{\mathbf{G}}}(r_n, r_m) \begin{bmatrix} \alpha_x(\omega) & 0 & 0 \\ 0 & \alpha_y(\omega) & 0 \\ 0 & 0 & \alpha_z(\omega) \end{bmatrix} \mathbf{p}_m \quad (1)$$

where $\alpha_\eta(\omega)$ is frequency dependent polarizability of NP along the η-direction, η is **x**, **y**, or **z**; $\mathbf{G}(\mathbf{r}_n, \mathbf{r}_m)$ is the dyadic layered medium Green's function matrix that gives the relationship between each component of the electric field vector at $\mathbf{r}_n$ and the oscillating electric dipole located $\mathbf{r}_m$. For the complete formulation of LMGFs, the reader is referred to [11].

Surface plasmon resonance occurs when the dipole moment of a single NP becomes equal to the induced dipole moment on that NP due to all the other dipoles. Using (1) and the fact that any vector in 3D space can be written as a combination of 3 orthogonal unit vectors, we can build three independent dispersion modes: one longitudinal and two transverse as

$$1 - \alpha_\eta(\omega) \sum_{n=1}^{M-1} G_{\eta\eta}(r_0, r_n) = 0, \qquad (2)$$

where $\mathbf{r}_n = nd\mathbf{x}$, assuming $\mathbf{r}_0$ is located at the origin, $\boldsymbol{\eta}$ is $\mathbf{x}$ for the longitudinal, $\mathbf{y}$ for the first transverse, or $\mathbf{z}$ for the second transverse mode. For a chain of M metal NPs, (2) becomes a set of M coupled equations in the M unknown moments of NPs. One can put these equations in a matrix form as explained in [3] and calculate resonance frequencies for which the matrix coupling the dipoles is singular. For the complete procedure, reader is referred to [3]. Replacing free space Green's functions with layered medium Green's functions is not enough to extend CDA to layered media; the polarizability of NPs should be handled appropriately as well: reflection terms of the layered medium Green's function should be subtracted from α.

III. NUMERICAL RESULTS

In [5,7,9], *Crozier et al.* present a systematic study on the dispersion relations of a metal nanoparticle chain fabricated on top of an indium tin oxide coated (ITO) glass slide. For the experiment, they use cylindrical gold nanoparticles with heights of 55 nm, diameters of ~90 nm, and center-to-center distances of 140 nm along the length of the chain. The thickness of ITO-coating is 20 nm. In [5], they also apply CDA technique to calculate SPR modes: first they assume point dipoles exist in the air, second they assume point dipoles exist in the glass. They observe that experimentally obtained dispersion results lay in between those two cases.

We analyze the same structure theoretically using layered medium CDA (abbreviated as LM-CDA). For the optical constants of gold, the experimental values are used rather than the Drude model to avoid the concerns about the selection of the appropriate values for plasmon and relaxation frequencies. We model cylinders as ellipsoids and calculate their polarizability using (2). The refractive indices of glass, ITO and air are assumed to be 1.51, 1.45 and 1, respectively and the procedure described in the previous section is followed on the complex ω domain using 20 NPs. Fig. 1 compares experimentally (dots and crosses) [5] and theoretically (lines) obtained dispersion relations. Compared to the classical CDA solutions [5], LM-CDA provides more accurate results. Both transverse modes interact strongly with the light line. Maximum propagation length for the first transverse mode is about 1μm, which is slightly higher than the case where NPs are situated in air. This means that we can increase the surface plasmon propagation length, supported by the plasmonic waveguide, based on the constructive backscattering phenomenon.

We repeat the same numerical study for the silver NPs and conclude that silver NP chain support longer propagation lengths. More detailed analysis of these results will be discussed at the conference.

IV. CONCLUSIONS

We implement layered medium dyadic Green's functions to obtain the dispersion relations for nanoparticle structures embedded in multilayered media. The polarizability of metal nanoparticles is approximated analytically by taking multilayered medium into account. We numerically show the existence of two different transverse modes. Both of these transverse modes strongly couple with the light line. Propagation lengths of 1μm are possible.
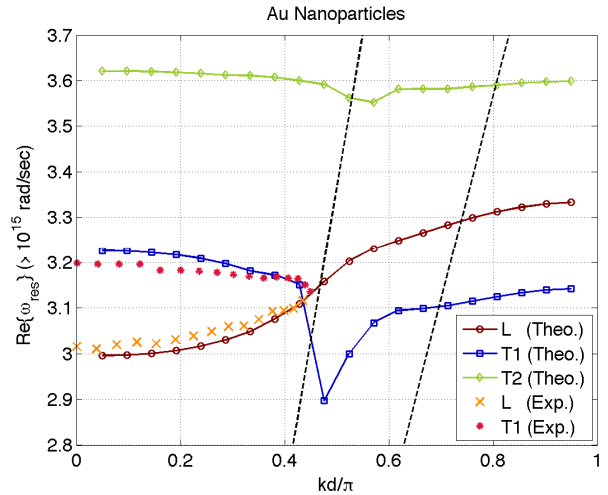

Figure 1 Experimentally (dots and crosses) and theoretically (lines) obtained dispersion curves. Dashed black lines depict light lines in air and glass.

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