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Substrate Effects onto Complex Modes and Optical Properties of 2D Arrays of Linear Trimers of Plasmonic Nanospheres

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***Abstract* – We first introduce the formulation of 2D periodic dyadic Green's function to account for all the field contributions required to thoroughly describe the physics of a 2D array of nanospheres on top of a multilayered substrate. Then, we analyze substrate effects onto complex modes and optical properties of 2D arrays of linear trimers of plasmonic nanospheres and show that Fano resonant features appear for oblique TM-polarized plane wave incidence illumination. These features are attributed to the forced excitation of free modes supported by the array, here computed via modal analysis. We observe strengthened Fano features due to the presence of the multilayered substrate.**

I. INTRODUCTION

Periodic arrays of nanoparticles have become important for many cutting-edge applications including the design of surface-enhanced Raman scattering sensors [1]-[2], Fano-resonance based sensors [3], nanowaveguides and nanoantennas [4]-[6]. This fact indeed motivates the studies behind wave propagation in periodic arrays of nanoparticles. Fabricated structures are usually deposited on top of multilayered substrates of some sort, and many theoretical works have yet neglected their effects on supported waves and optical properties (e.g., [7]). Effect of substrate has been taken into account in [8] where however periodicity effects have not been included. Both contributions have been instead accounted for in [9] for a 1D periodic array of dipoles. Regarding 2D periodic arrays of nanoparticles on layered substrates, scattering of light by such a system has been analyzed in [10]. Theoretical studies on the supported modes and on their optical properties have also been reported in [11] and [12], respectively. Efficient evaluation of periodic Green's function (GF) in multilayered media has been reported in [13]. In this paper, we first introduce the formulation employing 2D periodic dyadic GF for an array of nanoparticles located on top of a multilayered substrate and apply it to the evaluation of the optical properties and modes with complex wavenumber in an array of linear trimers of plasmonic nanospheres. This allows us to correlate Fano resonant features observable in the optical properties of such a structure under oblique TM-polarized plane wave to the forced excitation of free modes supported by the array. This result leads to a better understanding of wave propagation in fabricable arrays on multilayered substrate, opening up new ways to the development of optimized Fano-resonant sensors.

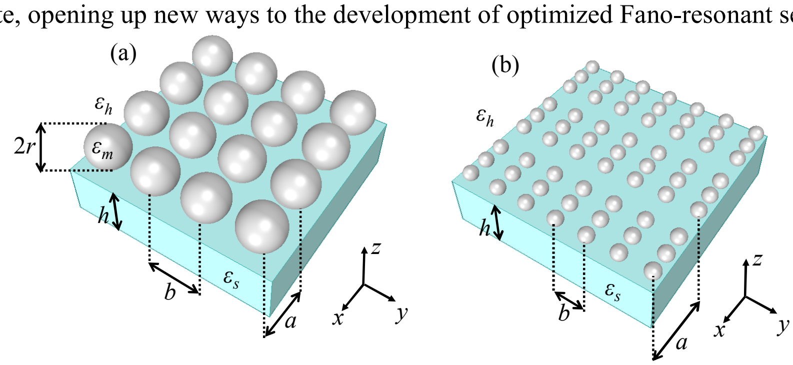

Fig. 1. 2D array of (a) nanospheres and (b) linear trimers on top of a substrate, with dimensions.

II. Formulation Employing 2D Periodic Dyadic Green's Function

Consider the 2D periodic array of nanospheres located at positions $\mathbf{r}_{mn} = \mathbf{r}_{00} + ma\hat{\mathbf{x}} + nb\hat{\mathbf{y}}$ on top of a substrate with thickness h and relative permittivity ε_s as in Fig. 1(a), with $\mathbf{r}_{00} = x_{00}\hat{\mathbf{x}} + y_{00}\hat{\mathbf{y}} + z_{00}\hat{\mathbf{z}}$ a reference location, $m, n = 0, \pm 1, \pm 2, \ldots$, and a and b the periods along the x and y directions, respectively. By resorting to the single dipole approximation (SDA) [4], each sphere has a dipole moment $\mathbf{p}_{mn} = \mathbf{p}_{00} \exp\left[i\mathbf{k}_{\mathrm{B}} \cdot \left(\mathbf{r}_{mn} - \mathbf{r}_{00}\right)\right]$, where $\mathbf{k}_{\mathrm{B}} = k_x\hat{\mathbf{x}} + k_y\hat{\mathbf{y}}$ is the Bloch wavevector, which also accounts for decay in case the wavenumbers are complex. The total electric field at a general position $\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$ is then given by

$$\mathbf{E}\left(\mathbf{r}, \mathbf{k}_{\mathrm{B}}\right) = \mathbf{E}^{\mathrm{inc}}\left(\mathbf{r}\right) + \left[\underline{\mathbf{G}}_0^{\infty}\left(\mathbf{r}, \mathbf{r}_{00}, \mathbf{k}_{\mathrm{B}}\right) + \underline{\mathbf{G}}_{\mathrm{sc}}^{\infty}\left(\mathbf{r}, \mathbf{r}_{00}, \mathbf{k}_{\mathrm{B}}\right)\right] \cdot \mathbf{p}_{00}, \tag{1}$$

where $\mathbf{E}^{\mathrm{inc}}$ is the incident electric field, $\underline{\mathbf{G}}_0^{\infty}$ is the dyadic GF in homogeneous environment and $\underline{\mathbf{G}}_{\mathrm{sc}}^{\infty}$ is the scattering GF that takes into account the effect of the substrate. We employ a spectral approach for the evaluation of $\underline{\mathbf{G}}_{\mathrm{sc}}^{\infty}$, decomposing each spectral plane wave to its TE and TM contribution. When computed at $\mathbf{r}_{00}$, the contribution from the $\mathbf{p}_{00}$ dipole in homogeneous environment has to be removed and thus we define the regularized GF $\underline{\breve{\mathbf{G}}}_0^{\infty}\left(\mathbf{r}_{00}, \mathbf{r}_{00}, \mathbf{k}_{\mathrm{B}}\right) = \lim_{\mathbf{r} \to \mathbf{r}_{00}} \left[\underline{\mathbf{G}}_0^{\infty}\left(\mathbf{r}, \mathbf{r}_{00}, \mathbf{k}_{\mathrm{B}}\right) - \underline{\mathbf{G}}_0\left(\mathbf{r}, \mathbf{r}_{00}\right)\right]$ that is not singular at $\mathbf{r} = \mathbf{r}_{00}$. $\underline{\mathbf{G}}_0^{\infty}$ in (1) and $\underline{\breve{\mathbf{G}}}_0^{\infty}$ are computed through the Ewald method for fast convergence [4]. The contribution from $\underline{\mathbf{G}}_{\mathrm{sc}}^{\infty}$ is computed spectrally as

$$\underline{\mathbf{G}}_{\mathrm{sc}}^{\infty}\left(\mathbf{r}, \mathbf{r}_{00}, \mathbf{k}_{\mathrm{B}}\right) = \frac{i}{2ab} \sum_{p=-\infty}^{+\infty} \sum_{q=-\infty}^{+\infty} \frac{1}{k_{z,pq}} \underline{\mathbf{G}}_{\mathrm{sc}}\left(z, \mathbf{k}\right) e^{i\mathbf{k}_{t,pq} \cdot \left(\mathbf{r} - \mathbf{r}_{00}\right)} e^{ik_{z,pq}\left|z - z_{00}\right|} \tag{2}$$

where $\mathbf{k} = \mathbf{k}_{t,pq} - k_{z,pq}\hat{\mathbf{z}}$, $\mathbf{k}_{t,pq} = \mathbf{k}_{\mathrm{B}} + (2\pi p / a)\hat{\mathbf{x}} + (2\pi q / b)\hat{\mathbf{y}}$, $k_{z,pq} = (k^2 - \mathbf{k}_{t,pq} \cdot \mathbf{k}_{t,pq})^{1/2}$, whose root is chosen such that $\mathrm{Im}\left(k_{z,pq}\right) > 0$, with $k = k_0\sqrt{\varepsilon_h}$ and k_0 is the free space wavenumber, and

$$\underline{\mathbf{G}}_{\mathrm{sc}}\left(z, \mathbf{k}\right) = \Gamma_{pq}^{\mathrm{TE}}\left(z\right)\hat{\mathbf{t}}_{pq}^{\mathrm{TE}}\left[\hat{\mathbf{t}}_{pq}^{\mathrm{TE}} \cdot \underline{\mathbf{G}}\left(\mathbf{k}\right)\right] + \Gamma_{pq}^{\mathrm{TM}}\left(z\right)\hat{\mathbf{t}}_{pq}^{\mathrm{TM}}\left[\hat{\mathbf{t}}_{pq}^{\mathrm{TM}} \cdot \underline{\mathbf{G}}\left(\mathbf{k}\right)\right] - \Gamma_{pq}^{\mathrm{TM}}\left(z\right)\hat{\mathbf{z}}\left[\hat{\mathbf{z}} \cdot \underline{\mathbf{G}}\left(\mathbf{k}\right)\right], \quad z_s < z < z_{00} \tag{3}$$

with z_s denotes the boundary location between substrate and array and $\underline{\mathbf{G}}\left(\mathbf{k}\right)$ is computed as described in [14]. For $z > z_{00}$, (3) should be computed as $\underline{\mathbf{G}}_{\mathrm{sc}}\left(z_{00}, \mathbf{k}\right)$. In (3), $\hat{\mathbf{t}}_{pq}^{\mathrm{TM}} = \mathbf{k}_{t,pq} / k_{t,pq}$, $\hat{\mathbf{t}}_{pq}^{\mathrm{TE}} = \hat{\mathbf{t}}_{pq}^{\mathrm{TM}} \times \hat{\mathbf{z}}$ are the unit vectors along the directions of transverse electric field components for TM and TE, and and $\Gamma_{pq}^{\mathrm{TM/TE}}$ the reflection coefficients for each TM and TE spectral wave. Note that the formulation is general and allows for the treatment of any kind of stratified substrate as well as clustered arrays.

III. Numerical Results Pertaining to a 2D Periodic Array of Linear Trimers on a Substrate

We consider here a 2D periodic array of linear trimers of nanospheres as in Fig. 1(b) and adapt the formulation in Sec. II accordingly. We report in Fig. 2 the absorption coefficient computed as in [15] (denoting the power dissipated in a unit cell) versus frequency and angle of incidence in two cases: (i) array in glass, i.e., $\varepsilon_s = \varepsilon_h = 2.25$; (ii) array in glass on top of a substrate with $\varepsilon_s = 10$ and thickness h = 50 nm. We also compute the free modes with complex wavenumber $\mathbf{k}_{\mathrm{B}} = k_x\hat{\mathbf{x}}$ supported by the array, and the ones that are phase-matched to the incoming plane wave (i.e., forced excitation) have been reported as dashed black lines in Fig. 2 as $\theta = \arcsin\left[\mathrm{Re}\left(k_x\right) / k\right]$. When dealing with the array in homogeneous environment, Fano features appear as absorption peaks around 700 THz for incident angles larger than 15 degrees. When the substrate is introduced, we observe two main effects: First, the Fano feature correspondent to the one observed in glass (slightly red shifted as one would expect) is strengthened;

second, a new Fano feature is observed around 550 THz, even for normal incidence. This is an important result as in the case in Fig. 2(a) material losses damp the Fano feature for small incident angles, which are restored in loss-compensated systems (not shown).

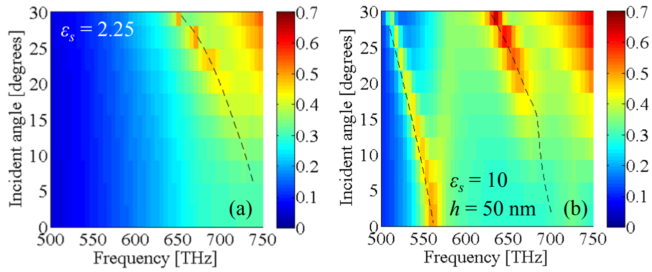

Fig. 2. Absorption coefficient for an array of linear trimers as in Fig. 1(b) with (a) $\varepsilon_s = 2.25$ and (b) $\varepsilon_s = 10$ with thickness h = 50 nm. Silver nanospheres are modeled with Palik data [16] with $r = 25$, $a = 210$, $b = 75$ (in nm), distance between nanospheres' centers within a unit cell along x is 60 nm, and $\varepsilon_h = 2.25$.

IV. Conclusion

We have applied SDA for 2D periodic arrays of nanospheres using the periodic dyadic GF for a multilayered substrate to the analysis of 2D arrays of linear trimers. We have found that the use of a substrate strengthens Fano features otherwise damped by the losses in the system.

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