

## Time - Domain Analysis of Surface Charge Distribution on Metallic Nanoparticles

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Abstract: Electromagnetic fields near metallic nanoparticles are analyzed by using a boundary integral equation method in complex frequency domain. The solution in time domain can be obtained by using fast inversion of Laplace transform. We investigate the time response of the surface charge distribution and the electromagnetic fields near metallic nanoparticles.

## 1. Introduction

For developing microfabrication technologies and ultra-high density recording, it is important to analyze electromagnetic fields near nanoscale objects<sup>[1]</sup>. In this paper, we investigate the electromagnetic fields near metallic nanoparticles with an integral equation and fast inversion of Laplace transform (FILT)<sup>[2]</sup>. Surface charge distribution and the electromagnetic field are discussed.

## 2. Formulation

When the object dimensions are much smaller than the incident wavelength, unknown surface charge density of the object is given by the following boundary integral equation in complex frequency domain<sup>[3]</sup>,

$$\hat{\sigma}(\mathbf{r}, s) - \frac{\hat{\lambda}}{2\pi} \oint_S \hat{\sigma}(\mathbf{r}', s) \frac{\mathbf{n} \cdot (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} dS' = 2\varepsilon_0 \hat{\lambda} \mathbf{n} \cdot \mathbf{E}^i \hat{f}(s), \quad (1)$$

where

$$\hat{\lambda} = \frac{\varepsilon(s) - \varepsilon_0}{\varepsilon(s) + \varepsilon_0}, \quad (2)$$

$\hat{\sigma}$  is the unknown surface charge density,  $\mathbf{n}$  is the unit vector normal to the surface of the object,  $\varepsilon(s)$  is the dielectric permittivity, and  $\hat{f}(s)$  is the image function of the incident wave.

The unknown electric charge density is expanded in an appropriately chosen set of basis functions  $\hat{g}_i$ , such as

$$\hat{\sigma}(\mathbf{r}, s) = \sum_{i=1}^N a_i \hat{g}_i(\mathbf{r}, s), \quad (3)$$

where  $a_i$  is the unknown expansion coefficient. The integral equation is discretized by using Eq. (3) and the testing function  $\hat{t}_j$ , such as

$$\sum_{n=1}^N A_{jn} a_n = F_j, \quad j = 1, 2, \dots, N, \quad (4)$$

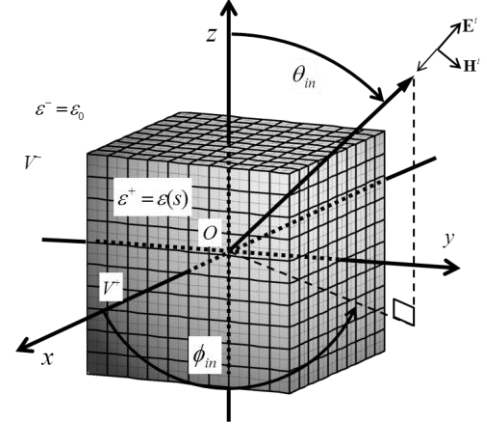


Figure 1. Geometry and coordinate systems.

where

$$F_j = 2\varepsilon_0 \hat{\lambda} \oint_S \hat{t}_j(\mathbf{r}, s) \mathbf{n} \cdot \mathbf{E}^i \hat{f}(s) dS, \quad (5)$$

$$A_{ji} = \oint_S \hat{t}_j(\mathbf{r}, s) \hat{g}_i(\mathbf{r}, s) dS - \frac{\hat{\lambda}}{2\pi} \oint_S \hat{t}_j(\mathbf{r}, s) \oint_S \hat{g}_i(\mathbf{r}', s) \frac{\mathbf{n} \cdot (\mathbf{r} - \mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|^3} dS' dS. \quad (6)$$

The unknown surface charge density obtained by the integral equation in complex frequency domain can be transformed into the time domain by using fast inversion of Laplace transform,

$$\begin{aligned} \sigma(\mathbf{r}, t) &= \frac{1}{2\pi j} \int_{\gamma-j\omega}^{\gamma+j\omega} \hat{\sigma}(\mathbf{r}, s) E_{st}(st, \alpha) ds \\ &= \frac{e^\alpha}{t} \sum_{m=1}^{M-1} F_m, \end{aligned} \quad (7)$$

where

$$F_m = (-1)^m \text{Im} \left[ \hat{\sigma} \left\{ \mathbf{r}, \frac{\alpha + j(m-0.5)\pi}{t} \right\} \right]. \quad (8)$$

Since the series is alternating, convergence can be faster by adding the Euler transformation terms,

$$\sigma(\mathbf{r}, t) = \frac{e^\alpha}{t} \left( \sum_{m=1}^{M-1} F_m + 2^{-(p+1)} \sum_{q=0}^p A_{pq} F_{M+q} \right), \quad (9)$$

where

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$$A_{pp} = 1, A_{pq-1} = A_{pq} + \frac{(p+1)!}{q!(p+1-q)!}, \quad (10)$$

$\alpha$  is the approximated parameter,  $M$  is the truncation number, and  $p$  is the truncation number of the Euler transformation.

### 3. Computational Results

Figure 1 shows the geometry of a nanoscale object and coordinate system. The object is a cube whose side is 10 nm. The medium is gold and the dielectric permittivity in the complex frequency domain is assumed to be the Lorentz-Drude model. The angles of the incident wave are  $\phi_{in} = 0^\circ$  and  $\theta_{in} = 0^\circ$ . The observation point is at  $x = 6$  nm and  $y = z = 5$  nm.

Figure 2 shows the wavelength characteristics of the electric field near the object. The incident field is a sinusoidal plane wave with the amplitude of 1.0 V/m. The computational result is obtained by the boundary integral equation. The resonance wavelength for which the electric field becomes the maximum is 555 nm in the range of 200 nm to 850 nm.

We suppose that a sinusoidal pulse with the amplitude of 1.0 V/m and the 1.5 period impinges on the cube. Figure 3 shows the time domain responses of the electric total field. The wavelength of the incident wave is chosen as 200, 555 and 850 nm from the computational result of Figure 2. For 200 and 850 nm, we can confirm that the amplitude of the scattered wave attenuates precipitously after the pulse passes through the object. For 555 nm, the amplitude of the scattered wave attenuates gently.

Figure 4 shows the surface charge distribution at 3.2 and 3.9 fs. The wavelength of the incident wave is 555nm. The plus and minus electric charges are distributed on the cube, and especially induced on the corners of the cube. As time passes, the plus and minus electric charges turn over the distribution on the surface of the scatterer.

### 4. Conclusions

We analyzed the surface charge distribution and the time response of the electromagnetic field near the surface of cubic metallic nanoparticles. Selecting the resonance wavelength, the amplitude of the scattered wave attenuates slowly after the pulse passes the object.

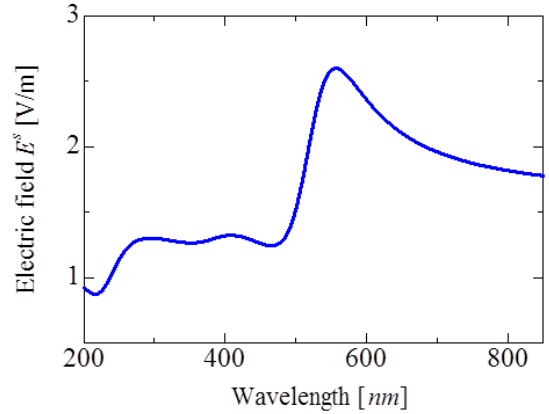


Figure 2. Wavelength characteristics of the electric total field.

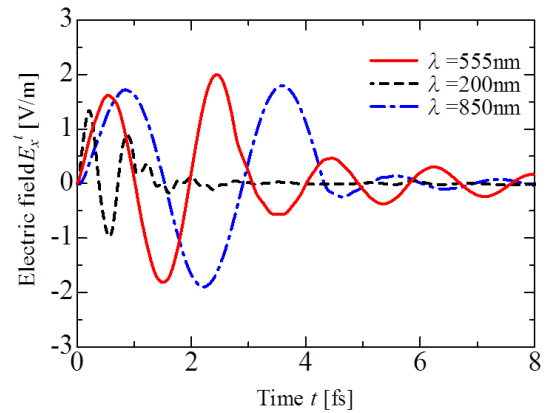


Figure 3. Time domain responses.

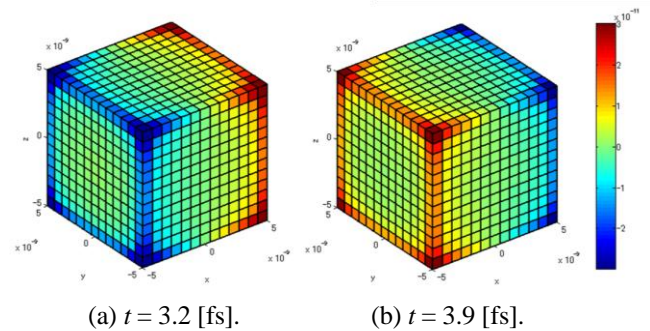


Figure 4. Surface charge distribution.

### 5. Acknowledgements

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### 6. References

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