L-10

Optimization for Rotational Control of Molecular Motors

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Abstract: Molecular devices are regarded as ultimate small machines and introduce the concept that one molecule operates like a machine. A molecular motor which consists of a molecule with an electric dipole is one of the molecular devices. We analyze electromagnetic characteristics of the molecular motor by using an integral equation method and fast inverse Laplace transform (FILT)[1][2], and investigate the way to control the rotation.

1. Introduction

Studies of molecular devices and machines are actively pursued in a nano-scale research area[3]. A molecular motor which consists of a molecule with an electric dipole is one of the molecular devices. The motion of a molecular motor is controled by the impressed electric field. To observe the motion of the molecular motor more easily, the new model using a gold nano sphere has been proposed recently[4].

We discuss surface charges on the nano sphere and the induced electric dipole moment of the molecular motor due to the impressed electric field.

2. Formulation

2.1 BIEM-FILT

When the object dimension is much smaller than the incident wavelength, unknown surface charge density of the object is given by the following boundary integral equation in the complex frequency domain[1],

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

where

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

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

$$\sigma(\mathbf{r},t) \approx \frac{e^{\alpha}}{t}\left(\sum_{m=1}^{M-1}F_m + 2^{-(p+1)}\sum_{q=0}^{p}A_{pq}F_{M+q}\right), \quad (3)$$

where

$$F_m = (-1)^m \,\mathrm{Im}\left[\hat{\sigma}\left\{\mathbf{r}, \frac{\alpha + j(m-0.5)\pi}{t}\right\}\right], \quad (4)$$

$$A_{pp} = 1,\ A_{pq-1} = A_{pq} + \frac{(p+1)!}{q!(p+1-q)!}, \quad (5)$$

$\varepsilon(s)$ is the dielectric permittivity, $\hat{f}(s)$ is the spectrums of the incident wave. α is the approximate parameter, M is the truncation number, and p is the truncation number of the Euler transformation.

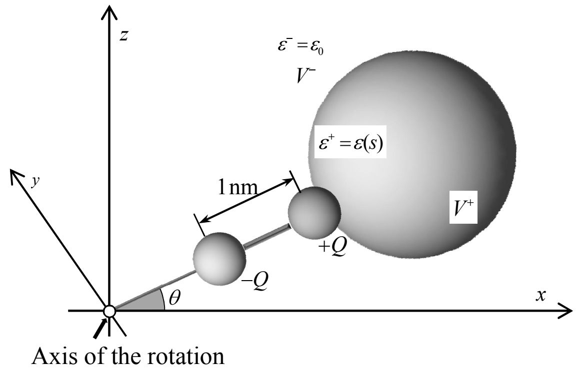

Figure 1. Coordinate system.

2.2 Motion equation

To analyze the movement of the molecular motor, the following motor equation is considered,

$$\frac{d^2\theta_{(t)}}{dt^2} = \frac{N_{-z}+N_{+z}}{m_-r_-^2 + m_+r_+^2 + (m_- + m_+)h^2}, \quad (6)$$

where

$$\mathbf{N}_{\pm} = \mathbf{d}_{\pm} \times Q_{\pm}\mathbf{E} = N_{\pm x}\mathbf{a_x} + N_{\pm y}\mathbf{a_y} + N_{\pm z}\mathbf{a_z}, \quad (7)$$

Eq.(6) is transformed into the complex frequency domain, such as

$$\Theta_{(s)} = \frac{\theta_0 s}{s^2 + \dfrac{E(Q_-d_- + Q_+d_+)}{m_-r_-^2 + m_+r_+^2 + (m_- + m_+)h^2}}, \quad (8)$$

where $m_{\pm}$ is the mass of the electric charge, $r_{\pm}$ is the length between the gravity center of the molecule and the electric charge, h is the length between the gravity center and the axis of the rotation, and $\mathbf{d}_{\pm}$ is the length between the axis of the rotation and the electric charge.

3. Computational Results

We set the molecule near the sphere whose radius is 5 nm. The total length of the molecule is 1 nm and the dipole moment of the molecule is 10 Debye. Figure 2 shows the surface charge distribution on the sphere. In the case of Figure 2 (a), the source is only the dipole of the molecule. It is obvious that the minus charges are induced on the surface

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patches close to the molecule, and the plus charges are induced on the other patches. When the sources are the molecule and the impressed electric field whose amplitude is 8 MV/m, the surface charge of the sphere is distributed as in Figure 2 (b). The impressed electric field affects the charge distribution.

Figure 3 shows the electric dipole moment of the molecular motor when the intensity of the impressed electric field is changed. The dipole moment keeps an almost constant value when the impressed electric field is less than 100 kV/m. The constant value is mainly determined by the dipole of the molecule.

When the circular polarized light is incident on the sphere, the electric dipole moment of the molecular motor is shown in Figure 4. The value of the electric dipole moment vibrates. In the case of the static electric field, the value of the electric dipole molecule converges to 37 Debye.

Here, the molecular motor is rotated by the impressed electric field. The starting value of the rotating angle is 20 deg. Figure 5 shows the time domain response of the rotating angles. The computational result by using the finite difference method and the computational result indicated by using FILT are in a good agreement.

4. Conclusions

The electric dipole moment of the molecule and the sphere for visualization were investigated. We showed that the strong electric field more than 10^5 order influenced the electric dipole moment of the molecular motor.

5. Acknowledgements

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6. References

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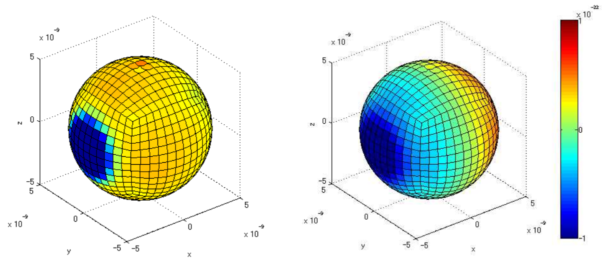

(a) (b)

Figure 2. Surface charge distributions of the sphere.

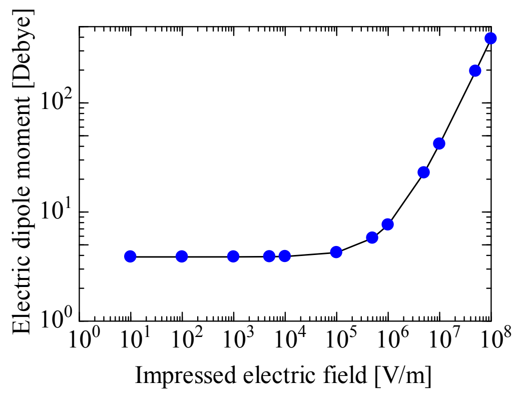

Figure 3. Electric dipole moment.

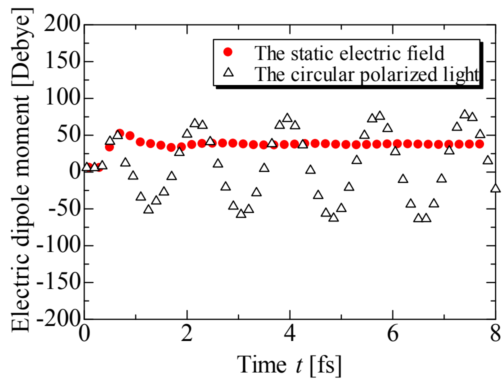

Figure 4. Time domain response of the electric dipole moment.

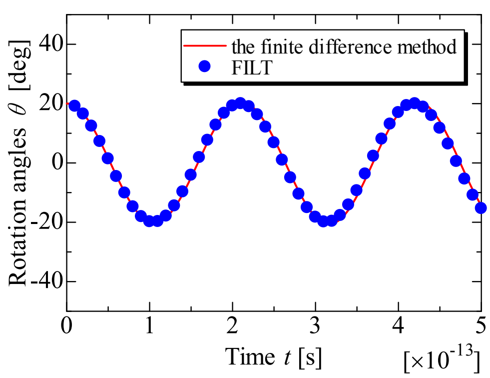

Figure 5. Time domain response of the rotating angles.