The motion of nanoparticles under the non-conservative forces mediated by surface plasmon polaritons

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Abstract. We have developed the theoretical and numerical modelling of nanoparticle dynamics near planar metallic interface under light radiation. Using our model, we employed the Green's function formalism to simulate the dynamics of nanoparticles under the action of surface plasmon polariton mediated optical forces. By varying the illumination conditions, we determined the different regimes of motion, such as surface attraction and repulsion, and optical pulling regime. We showed that the topology of the trajectories dramatically change, when the surface plasmon polaritons are excited.

1. Introduction
Nowadays optical tweezing and light manipulation of nanoobjects became one of the common tools in modern optical instrumentation [1]. The unique opportunities for non-invasive control of objects at the nanoscale made it highly prospective for biological and biochemical applications [2]. Currently, the active studies in the field of optical forces are devoted to the forces generated via momentum exchange with surface waves [3-5]. This approach gives new perspectives for developing methods of nanoparticles transport and optical sorting. While almost all the studies are devoted to stationary computations of optical forces, the exact dynamics of the nanoparticles motion in the presence of the substrate is not studied yet. In our work, we suggest the dynamical model of nanoparticle motion near the interface between two media. We apply the model for simulating nanoparticle trajectories near metallic interfaces, which support surface plasmon polariton (SPP) waves. Using the developed model, we show the different regimes of the nanoparticle dynamics due to SPP modes interaction, which strongly depends on the illumination conditions.

2. Forces acting onto a point dipole near interface
We start by examining the problem in the dipole approximation when the nanoparticle size is smaller than the wavelength and typical scales of electric field variations. We consider a spherical dielectric nanoparticle with permittivity \( \varepsilon_p \) and radius \( R \) located inside a medium with permittivity \( \varepsilon_m \). The particle is placed at the height \( z_0 \) above a substrate with permittivity \( \varepsilon_s \), as shown in Figure 1. The incident wave with wavelength \( \lambda = 2\pi/k_1 \) impinges onto the surface at the angle \( \theta \).
Figure 1. (a) The inset depicts the geometry of the problem: a dielectric particle is located near silver planar interface. Incident electromagnetic wave is propagating from the upper half-space.

Assuming that the nanoparticle is small in comparison to the wavelength, $R \ll \lambda$, one can consider it as a point electric dipole with polarizability $\alpha_0 = i6\pi\varepsilon_0 a_1/(k_1\sqrt{\varepsilon_m})^3$, which is given by the Mie theory, where $a_1(\varepsilon_p, \varepsilon_m, k_1, R)$ is the scattering coefficient [8]. The averaged optical force which is acting onto a particle located in $\mathbf{r}_0$ in an arbitrary electric field $\mathbf{E}^{\text{loc}}$ can be written as [6]

$$ F_j = \frac{1}{2}\text{Re}[\mu_i \mathbf{E}^{\text{loc}}], $$

(1)

where Einstein summation notation was used and $\mu = \alpha_0 \mathbf{E}^{\text{loc}}$ is the induced dipole moment. The local electric field acting on a particle may be written as $\mathbf{E}^{\text{loc}} = \mathbf{E}^{\text{inc}} + \mathbf{E}^{\text{ref}} + \mathbf{E}^{\text{scat}}$, where $\mathbf{E}^{\text{scat}}$ is scattered dipole field which includes the field induced by local fields generated in the substrate. The last component may be found to be

$$ \mathbf{E}^{\text{scat}}(\mathbf{r}) = \omega^2 \mu_0 \hat{G}^R(\mathbf{r}, \mathbf{r}_0)\mu, $$

(2)

where $\omega$ is the frequency of the incident wave, $\mu_0$ is the vacuum permeability and $\hat{G}^R(\mathbf{r}, \mathbf{r}_0)$ is the dyadic Green’s functions for the reflected dipole fields near planar interface [6]. Self-action of the dipole on itself may be taken into account by introducing the effective polarizability

$$ \tilde{\alpha} = \alpha_0 \left[ I - \alpha_0 \omega_0 \mu_0 \hat{G}^R(\mathbf{r}_0, \mathbf{r}_0) \right]^{-1}, $$

(3)

where $I$ is the unity tensor. In this particular case $\hat{G}^R(\mathbf{r}_0, \mathbf{r}_0)$ has only diagonal terms. Due to the symmetry of the problem $\tilde{\alpha}_{xx} = \tilde{\alpha}_{yy}$. After that the dipole moment can be calculated directly as $\mu = \tilde{\alpha}(\mathbf{E}^{\text{inc}} + \mathbf{E}^{\text{ref}})$.

Figure 2. Lateral (left) and normal to the substrate (right) components of the force for a particle with $\varepsilon_p = 3$ and $R = 15 \text{ nm}$ above silver substance for different gaps. Dielectric permittivity of silver is taken from [9] and incident angle is $\theta = 35^0$. For wavelengths $\lambda > 340 \text{ nm}$ SPP effects take place. Values are normalized to the radiation pressure force $F_0 = \frac{1}{2}k_1|\mathbf{E}^{\text{inc}}|^2\text{Im}(\alpha_0)$ acting on the spherical nanoparticle in the absence of a substrate.

Analysis of the optical force (1) shows that a so-called recoil force regime is possible [4]. It is an effect of emergence of a pulling force towards the light source, in this particular case it means $F_x < 0$. 
The physical background of this effect is in the directional radiation of surface plasmon waves. The important conditions are i) excitation of SPP wave, and ii) small gap between particle and the metallic surface. Moreover, the less particle size is, the more significant is the SPP contribution. The most efficient angle to observe the largest negative pulling force is $\theta = 35^\circ$ [4].

3. Dynamic simulation results and discussions

In this section we find the specific parameters corresponding to the overall pulling force. For further simulations particle radius was chosen $R = 15$ nm. To indicate the parameters of potentially different regimes of motions, the optical force was calculated within the expression (1). In Figure 2 it is shown that for $\lambda \geq 340$ nm SPP effects are important, and for significantly small gap $R$ gets negative. For further simulation of nanoparticle dynamics, two wavelength were chosen: $\lambda_1 = 320$ nm for a non-SSP regime and $\lambda_2 = 340$ nm for a strong SSP regime. The equation of motion for the particle is

$$m\ddot{\mathbf{r}} = \frac{1}{2} \text{Re} [\mu'_i \mathbf{E}^\text{loc}_E (\mathbf{r})] - \gamma \dot{\mathbf{r}},$$

(4)

where $m$ is the mass of the particle, and $\gamma$ is a phenomenological viscosity damping parameter. Differential equation (4) was solved numerically for $\lambda_1$ and $\lambda_2$ with different initial particle positions $z_0$. The laser power was chosen to be 100 mW and with the beam cross section of $10 \text{ nm}^2$, which defines the amplitude $E^\text{inc}$ of the incident wave.

The solution of the dynamical equation (4) is presented in Figure 3. One can see that the topology of the trajectories are dramatically changed when the wavelength of the incident light is changed from $\lambda_1$ to $\lambda_2$. In the non-plasmonic regimes the nanoparticle moves along the direction of light incidence, finally getting into the position of equilibrium with respect to vertical coordinate at approximately 30 nm height. At the same time in the regime of SPP excitation (see Figure 3, right panel) one can see that nanoparticle is first pulled, being displaced along the negative horizontal direction. Then it also ends at the z-equilibrium position around 45 nm above surface.

![Figure 3](image-url) The nanoparticle trajectories in the non-plasmonic (left) and plasmonic (right) regimes for different initial height of nanoparticle above the interface. The color denotes the time during the nanoparticle motion.

4. Conclusions

In this work we show that nanoparticle dynamics placed close to the metallic interface is significantly affected by the excitation of surface plasmon polariton modes. Depending on the condition of the exciting plane wave incidence one can achieve different conditions of SPP generation, and, in particularly, one can see the pulling action and displacement of nanoparticle in the direction opposite to the direction of light incidence.

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