Electrical interaction between nanoparticle and surface of material

C. Summueang¹, S. Boonchui¹,*
¹Department of Physics, Kasetsart University, Bangkok, 10900, Thailand
*Corresponding author e-mail: fscistb@ku.ac.th

Abstract. We identify the interaction between nanoparticle and surface of material in the presence of an electric field. For theoretical calculation, we use the dyadic green function that includes with the method of image dipoles to analyze electrical interaction. We find that the electric field and the interaction potential which depend on the dielectric constant and surface roughness of material. Our numerical results demonstrate the electric field and the interaction potential which corresponds to the Van der Waals interaction and can be used to determine charges distribution on nanoparticle and surface of material.

1. Introduction

Particles in nanometer-scale were influenced in the presence of an electric field that attracts on surface of metallic material and caused an impact of the electrical problem between nanoparticle and surface material that was acquired the interaction when nanoparticle is located close metallic substrate [1]. The interaction is related to electrical dipole moment and corresponds to the Van der Waals interaction [2,3].

We shall concentrate to our theoretical attention on the problem of nanoparticle in the colloidal state model and the interaction between a nanoparticle and the surface of a solid combined with the theoretical framework based on the physical properties of the polarization and magnetic Casimir-Polder interaction [4].

Particle colloidal behaviour is then compared to that of both isotropic and anisotropic minerals in order to gain further information regarding the surface charge distribution [5]. We have shown that it possible to explain the contamination of nanoparticle on the metallic substrate by using the dyadic Green’s function [6] include with the method of images approach. By replacing the molecular particle–surface interaction with a molecular–image interaction, the image molecule due to the surface roughness [7] and the dielectric constant of the substrate. A magnitude of image molecule is proportional to the surface roughness and dielectric constant. This well-established technique can account for the force of attraction between a charge and an uncharged dielectric medium, Van der Waals interactions between molecules and surfaces. [8]

In this work, the main goal of our work is to analyze with numerical calculation the interaction potential from the consideration of the effect from dielectric constant to display through electric field graphs and predict charges distribution on particle and metallic material by comparing with the theoretical results. To compare with experimental results, we regard polarization of surface (surface roughness) and demonstrate our results through the interaction potential that are corresponding to Van der Waals interaction.
2. Theoretical calculation

We will present a theoretical approach for calculating the interaction between a finite-size nanoparticle of an arbitrary shape and the surface of a solid. Let us consider a nanoparticle located close to the metallic surface. The particle is situated in the medium with the dielectric constant  $\varepsilon_m$ that fills the half space  $z > 0$, the surface with dielectric constant  $\varepsilon_s$. The metallic surface is XY plane. The center of the particle is located at the point $\vec{R}_p = (0,0,d)$. To analyze the interaction, the potential in the system can be presented as [1]

$$ U(d) = -\int_{V_p} d\vec{R}_p \vec{r} \cdot \vec{E} - U(d \to \infty) $$

(1)

In order to find the electric polarization and electric field, one can write the free energy of the system that includes with the internal energy density and the energy of the polarization density in the following form [4]

$$ E_f = \int_{V_p} d^3\vec{R}_p (U_{int} - \vec{P} \cdot \vec{E}) + \int_{\mathbb{R}^3} d^3\vec{R}_p W $$

(2)

The electric dipole moment corresponding to the ground state of the system can be found from

$$ \frac{\partial E_f (P_i)}{\partial P_i} = 0 $$

(3)

As a result of Eq. (3), one obtains the following connection between the dipole moment at the particle and the electric field

$$ P_i(\vec{R}) \approx X^{(p)}_{ij}(\vec{R}_p) E_j^{(0)}(\vec{R}) + A^{(p)}_{ij}(\vec{R}_p) E_j^{(0)}(\vec{R}) E_k^{(0)}(\vec{R}) E_j^{(0)}(\vec{R}) $$

(4)

To calculate the electric field with the Lippmann-Schwinger equation by using dyadic Green’s function method [9,10,11]

$$ E_i(P_j) = E_i^{(0)} + \frac{k_n^2}{\varepsilon_0} \int_{V_p} dR_p \vec{G}_{ij}(R_p, \omega) \cdot P_j(R_p) $$

(5)

The dyadic Green’s function that is used in Eq. (5) is divided into the direct and the indirect term in the following form [10,12]

$$ G_{ij}(\vec{R}, \vec{R'}, \omega) = G_{ij}^{(d)}(\vec{R}, \vec{R'}, \omega) + G_{ij}^{(i)}(\vec{R}, \vec{R'}, \omega) $$

(6)

In the surface of metallic material take into account the surface roughness. Thus, One can put the effect of polarization from the surface in Eq. (2) in the form [7]

$$ \vec{P}_s(\vec{r}) = \vec{p} b(\vec{r}) $$

(7)

and

$$ \vec{p} = \gamma_z \hat{z} \cdot \vec{E}_i + \gamma_x (\hat{x} \hat{x} + \hat{y} \hat{y}) \cdot \vec{E}_i $$

(8)
3. Result and Discussion

3.1. Electric field of the system without surface roughness consideration
In order to obtain the numerical calculation, let us consider nanoparticle as a square particle in the presence of an applied external electric field in Z direction that came close to the surface of metallic material. To verify the theoretical calculation that corresponded with theoretical results without surface roughness consideration, in Figs. 1-3 was shown electric field by contour plot with each substrate in different the dielectric constant. One can see that the dielectric constant increases with the increase of the image particle that rise the interaction between particle and substrate increases. Consequently, the interaction depends on the dielectric constant of the substrate [4].

![Figure 1](image1)

**Figure 1.** Electric field in the system from substrate I with $\varepsilon_s = 28$.

![Figure 2](image2)

**Figure 2.** Electric field in the system from substrate II with $\varepsilon_s = 57$.

![Figure 3](image3)

**Figure 3.** Electric field in the system from substrate III with $\varepsilon_s = 130$.

3.2. The experimental result and the interaction potential
The experimental result is shown in Fig.4, this is the probability of contamination of nanoparticle on the substrate. Due to the fact, that should be increased linearly according to the above mentioned. Thus, Let us consider the case when a nanoparticle interacts with a metallic substrate in the presence of surface roughness consideration and determine the interaction potential. The results of this calculation, are shown in Fig. 5. Obtained results are concentrated in substrate II that correspond to the experimental result. The potential depends on the dielectric constant and surface roughness and is not linear.
4. Conclusion
In our work, we have discussed the effect of the interaction potential between nanoparticle and the metallic substrate using the method of image in dyadic Green’s function. First, we discuss the case without surface roughness displaying through the field plots. According to the theory, the field depended on that the dielectric constant of each substrate was increased. As it has shown from contour graphs, the images particle under substrate with a high dielectric constant will more intensity than low dielectric constant. Because of high dielectric constant material is more the ability of the material to store electrical energy than the others. When we include with roughness consideration, one can see the decreasing of probability in substrate II and corresponds to the potential in Fig. 5 which are caused by surface morphology. The interaction is in addition to dielectric constant dependent on the substrate, moreover physical properties of the substrate is significant to investigate.

5. Reference
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