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Ponderomotive forces in the system of two nanoparticles

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Abstract.

Mechanical consequences of electromagnetic interaction of two nanoparticles have been studied theoretically. It has been shown that local field enhancement effect, which causes appearance of the local field gradients, can lead to ponderomotive forces acting on the nanoparticles. Distribution of the local field in the system has been calculated and ponderomotive forces directions and values were evaluated. It has been shown that in the system of two different-sized nanoparticles the forces act mainly on the surface of bigger nanoparticle and for some systems its value may acquire up to several tens of nanonewtons. Possible application of the results to study of biological systems has been also discussed.

Keywords: nanoparticle; near-field interaction; local field enhancement; local field gradient; ponderomotive forces.

1. Introduction

System of two nanoparticles is the simplest nano-sized system, which is used for understanding the processes occurring at the nano-scale. In such system the interactions can be described analytically, which is needed for analysis of the system properties caused by the interactions inside it. Interaction between two nanoparticles leads to the adsorption of one particle at the another one due to Van der Waals or Casimir forces [1,2]. This interaction can have both attractive and repulsive parts caused by nonlinear polarizability of small particles [3,4]. The sign of the force can be changed from attractive to repulsive by suitable choice of interacting materials immersed in a fluid as it was discussed in [5]. Moreover, it was demonstrated that self-consistent electrodynamic interaction between two different-sized nanoparticles can lead to the repulsive part in adsorption potential [6]. The forces may also become repulsive for a special system geometry [7,8] or for interacting magnetic bodies [9]. Anyway, the forces lead to formation of the stable system of two nanoparticles which under action of external electromagnetic radiations (it can be daylight, for example) usually demonstrate the local field enhancement effect [10-12]. Then, at nearest of so-called ‘hot spots’ (area with strong local field) rather strong gradients of the local field can be observed [13,14]. If the polarization is distributed over the surface of the particle (which can be observed, for example, in the colloidal solutions of nanoparticles), the ponderomotive forces caused by local field gradients acting on the dipoles occur. Development of the model for

description and calculation of the forces connected with such electromagnetic interaction is the main aim of this work.

2. The methods and main equations

Consider the system of two different-sized nanoparticles (Fig.1). The bigger nanoparticle consists of a core and a shell. Suppose the external light incidence to the system. The angle between the direction of light propagation and the system symmetry axis OZ is θ . In order to demonstrate the effect of the interparticle interaction we need to calculate the effective susceptibility [15] of the system under consideration. It is convenient to use the pseudovacuum Green function method [16]. Consider the medium consisting of the environment in which the small nanoparticle is embedded. Let the effective susceptibility of nanoparticle is $X_{ij}^{(p)}(\mathbf{R}, \omega)$.

Figure 1. The sketch of the system under the action of external illumination.

The electrodynamic Green function of environment is $G_{ij}^{(0)}(\mathbf{R}, \mathbf{R}', \omega)$. Then, using the method proposed in [16], the pseudovacuum Green function of the system ‘small nanoparticle-environment’ can be written as follows

$$G_{ij}^{(m)}(\mathbf{R}, \mathbf{R}', \omega) = G_{ij}^{(0)}(\mathbf{R}, \mathbf{R}', \omega) -$$

$$-k_0^2 \int_{V_p} d\mathbf{R}'' G_{ik}^{(0)}(\mathbf{R}, \mathbf{R}'', \omega) X_{kl}^{(p)}(\mathbf{R}'', \omega) G_{lj}^{(0)}(\mathbf{R}'', \mathbf{R}', \omega), \quad (1)$$

where the integration is over the small nanoparticle volume, $k_0 = \omega / c$.

As it was shown in [15] the effective susceptibility of big nanoparticle embedded in the pseudovacuum (the effective medium) described by Green function $G_{ij}^{(m)}(\mathbf{R}, \mathbf{R}', \omega)$ can be calculated according to

$$\Xi_{ij}^{(v)}(\mathbf{R}, \omega) = \left[\left(X_{ij}^{(v)}(\mathbf{R}, \omega) \right)^{-1} - k_0^2 \int_{V_v} d\mathbf{R}' G_{ji}^{(m)}(\mathbf{R}, \mathbf{R}', \omega) \right]^{-1}, \quad (2)$$

where $X_{ij}^{(v)}(\mathbf{R}, \omega)$ is the susceptibility of the big nanoparticle calculated without taking into account of self-action processes. It can be evaluated from the following equation [17]

$$X^{(p)}(\omega) = 3 \frac{(\epsilon_2 - \epsilon_m)(\epsilon_1 + 2\epsilon_2) + f_1(\epsilon_1 - \epsilon_2)(\epsilon_m + 2\epsilon_2)}{(\epsilon_2 + 2\epsilon_m)(\epsilon_1 + 2\epsilon_2) + f_1(2\epsilon_2 - 2\epsilon_m)(\epsilon_1 - \epsilon_2)}, \quad (3)$$

where a_2 is the outer radius, ϵ_1 and ϵ_2 are the core (of radius a_1) and shell dielectric functions, respectively. The core volume fraction is $f_1 = a_1^3 / a_2^3$.

For calculation of the local field intensity (including the ‘hot spots’) the equation of self-consistency (so-called Lippmann-Schwinger equation) [16] should be used

$$E_i(\mathbf{R}, \omega) = E_i^{(0)}(\mathbf{R}, \omega) -$$

$$-k_o^2 \int_{V_v} d\mathbf{R}' G_{ij}^{(m)}(\mathbf{R}, \mathbf{R}', \omega) \Xi_{jl}^{(v)}(\mathbf{R}', \omega) E_l^{(0)}(\mathbf{R}', \omega). \quad (4)$$

Then, the force acting to the big nanoparticle can be written as

$$F_i(\mathbf{R}) = \left(P_j(\mathbf{R}) \cdot \frac{\partial}{\partial x_j} \right) E_i(\mathbf{R}), \quad (5)$$

where $P_j(\mathbf{R}) = \Xi_{jl}^{(v)}(\mathbf{R}) E_l^0(\mathbf{R})$ is the polarization (density of the dipole moment) of the nanoparticle shell. Then, using (4) we obtain

$$F_i(\mathbf{R}) = \left(\Xi_{jk}^{(v)}(\mathbf{R}) E_k^0(\mathbf{R}) \cdot \frac{\partial}{\partial x_j} \right) \cdot \left[E_i^{(0)}(\mathbf{R}, \omega) - k_o^2 \int_{V_v} d\mathbf{R}' G_{is}^{(m)}(\mathbf{R}, \mathbf{R}', \omega) \Xi_{sl}^{(v)}(\mathbf{R}', \omega) E_l^{(0)}(\mathbf{R}', \omega) \right].$$

Taking into account that at the distances about characteristic linear dimension of the nanoparticle, the external field is rather constant, this equation may be reduced to the following one

$$F_i(\mathbf{R}) = -k_o^2 \Xi_{jk}^{(v)}(\mathbf{R}) E_k^0(\mathbf{R}) \cdot \int_{V_v} d\mathbf{R}' \frac{\partial}{\partial x_j} G_{is}^{(m)}(\mathbf{R}, \mathbf{R}', \omega) \Xi_{sl}^{(v)}(\mathbf{R}', \omega) E_l^{(0)}(\mathbf{R}', \omega). \quad (6)$$

Note, in (6) the differentiation is over the components of $\mathbf{R}$. The action of the force onto unit of the shell surface obviously can change the shell properties up to its destruction.

In the model of ellipsoid susceptibility homogeneous field tensor $\Xi_{jk}^{(v)}(\mathbf{R})$ does not depend on coordinate [18], i.e. $\Xi_{jk}^{(v)}(\mathbf{R}) \rightarrow \Xi_{jk}^{(v)}$. Then, the dependence of the force from (6) on coordinate has its origin from the local field distribution at the surface of big nanoparticle only – via the dependence of the Green

1 function $G_{is}^{(m)}(\mathbf{R}, \mathbf{R}', \omega)$ on $\mathbf{R}$ (see (6)). Remember that the external field
 2 $E_l^{(0)}(\mathbf{R}, \omega)$ is the constant in the near-field approximation. Then it can be
 3 obtained from (6)

$$4 \quad F_i(\mathbf{R}) = -k_o^2 \left(\Xi_{jk}^{(v)} \cdot \int_{V_v} d\mathbf{R}' \frac{\partial}{\partial x_j} G_{is}^{(m)}(\mathbf{R}, \mathbf{R}', \omega) \Xi_{sl}^{(v)} \right) E_k^{(0)} E_l^{(0)} . \quad (7)$$

5 As the ‘hot spots’ (the domains of strong local field) locations are defined
 6 by Green function dependence on $\mathbf{R}$, the forces acting to the big (shelled)
 7 nanoparticle will be concentrated at the hot spots.

8 **3. Results of numerical calculations**

9 In this section we represent the results of calculations of the mechanical
 10 force distribution, which appears in the system of two different-sized
 11 nanoparticles. As it was mentioned previously, the force is caused by the action
 12 of the local field gradient on the polarized object. Hence, the force gain its
 13 maximum values at the points of the highest field gradient. Typical local field
 14 distribution for system of two nanoparticles is shown in Fig. 2, others can be
 15 find e.g. in [19-20].

Figure 2. Distribution of local field in the system of the nanoparticle of 60 nm radius with 10 nm shell ($\epsilon_{core} = 2$, $\epsilon_{shell} = 4$) located close to the nanoparticle of 2.5 nm radius (left) and of 10 nm (right) with $\epsilon_{np} = 10.5 + 1.3i$ in the medium with $\epsilon_m = 1$. Section at the $y = 0$ (dotted line is the surface of the bigger nanoparticle). Note, for the system with smaller nanoparticle the field is much higher than 1.8. This area is shown by lines.

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2 It can be seen that the ‘hot spots’ and highest gradients are located at the
3 surface of the biggest nanoparticle, which is schematically shown in Fig. 3.
4 Hence, we present results of calculations as the distribution of tangential and
5 normal forces. Such presentation of results is convenient for their analysis and
6 understanding.

Figure 3. Sketch of the forces acted on the bigger nanoparticle in the system of two different-sized nanoparticles.

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2 As the main goal of the work is to reveal the possible presence of
3 mechanical forces in the system of two nanoparticles, we conducted calculations
4 for one system with following parameters: the bigger nanoparticle is of 60 nm
5 radius with the shell of 10 nm thickness and the smaller nanoparticle is of 2.5
6 nm radius without a shell. The dielectric constant of the bigger nanoparticle core
7 is 2, the one of the nanoparticle shell is 4, and the one of the smaller
8 nanoparticle is $10.5 + 1.3i$. The system is supposed to be located in the medium
9 with $\varepsilon_m = 1$. Results of calculations are presented in Fig. 4.

Figure 4. Distribution of tangential (left) and normal force (right) on the surface of the nanoparticle of 60 nm radius with 10 nm shell ($\epsilon_{core} = 2$,

$\epsilon_{shell} = 4$) located close to the nanoparticle of 2.5 nm radius with

$\epsilon_{np} = 10.5 + 1.3i$ in the medium with $\epsilon_m = 1$. Section at the $y = 0$.

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It can be seen, that indeed in the system the strong mechanical forces may appear close to the surface of bigger nanoparticle due to the local field redistribution and the nanoparticle polarization. However, the field of force is quite narrowly localized, which can be easily understood from the local field distribution described previously. The interesting result is that the forces are directed inside the bigger nanoparticle in different sides. Such force deforms the nanoparticle and may lead to its breakage when the stress caused by the force prevails the nanoparticle limit of strength. As it was mentioned above, the nanoparticles size and shape are the main parameters which influence on the local field distribution. However, for the non-spherical nanoparticles the model should be much more complicated. But we can apply the same model for the

system with nanoparticles of bigger sizes [21-22]. Results for the similar system with the radius of smaller nanoparticle of 10 nm are presented in Fig. 5. Note, the maximum force is about one order of magnitude smaller compared to the system with smaller nanoparticle in Fig. 4. These results are in good coincidence with previous calculations and well-known experimental facts, that local field enhancement effect is much stronger near smaller nanoparticles.

Figure 5. Distribution of tangential (left) and normal force (right) on the surface of the nanoparticle of 60 nm radius with 10 nm shell ($\epsilon_{core} = 2$, $\epsilon_{shell} = 4$) located close to the nanoparticle of 10 nm radius with $\epsilon_{np} = 10.5 + 1.3i$ in the medium with $\epsilon_m = 1$. Section at the $y = 0$.

4. Discussion: interaction between the virus and nanoparticle.

One of interesting possible applications of the described effect may be found in the nanobiomedicine. Last years the numerous studies of interaction between the viruses and nanoparticles are provided because of the interest to

1 develop the new methods of antiviral therapy. These studies shown, that the
2 interaction between the nanoparticles and viruses can be the reason of lost by the
3 virus its infectivity [21-27]. The effect is observed equally well for different
4 types of nanoparticles, which excludes the chemical reasons of the effect. As the
5 domains of high field mean the exist of gradients of the local field at the surface
6 of bigger nanoparticles, i.e. they are localized at the virus shell. The molecules
7 at the surface of virus contain the polar sites [28-29]. Consequently, the dipole
8 moments of the polar sites are under action of field gradients. It means that the
9 ponderomotive forces acting to these molecules arises. Hence, in such systems
10 the virus shell deformation or destruction may appear. This effect was
11 demonstrated, in particular, for interaction between the TiO_2 nanoparticles and
12 influenza viruses H1N1 type when the viral envelope was destructed for 15 min
13 of exposition [24]. In the work [22] numerous results of action of nanoparticles
14 to the viruses were analysed and was concluded that the interaction between
15 nanoparticles and viruses has a field nature and can be connected with local-
16 field enhancing effect. The results of similar experiments provided for the
17 system gold nanoparticles of different sizes and influenza virus H1N1 were
18 reported in our previous work [25]. We calculated the ponderomotive forces
19 arising in the virus shell of H1N1 under action of Gold nanoparticles (diameter
20 5-7 nm) with the method developed in the present work and obtained the value
21 of the force about 3-7 nN which is sufficient for destruction of virus shell. More

detail as experimental as theoretical investigations of virus-nanoparticle interactions will be made in the future works.

5. Conclusions

The local field enhancement effect and physical adsorption in nanosystems due to Van der Waals interaction are well-known phenomena in nanophysics. The model and calculations presented in the work show that as a consequence of such electromagnetic processes the ponderomotive forces acting on the nanoparticle appear. Obviously, that these forces need to be taken into account as they may lead to deformation or even destruction of nanoparticles in nanosystems. As it can be seen from the model, the forces depend on the local field gradient, which in turn depends on the nanoparticles sizes, shapes, and materials [21]. For example, as in systems with bigger nanoparticles the local field gradient is lower [22], the forces values in these systems are lower too.

Declarations

Availability of data and materials

All the model parameters are included in this article. Other details are available from the corresponding author on reasonable request.

Competing interests

The authors declare that they have no competing interests.

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Authors' contributions

VLys designed the study; VLoz developed the methods; NR conducted numerical calculations; NR and VLoz analyzed results and interpreted numerical data. All the authors drafted the manuscript.

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