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Radiation Forces on a Cluster of Spherical Nanoparticles in Visible Light Spectrum

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Abstract—The scattering of the electromagnetic waves by the spherical particles is discussed. Nanometer-sized dielectric spheres confined in a cluster are devoted to investigate the effect of the EM radiation on them. Incident wave is considered to be in visible light spectrum which facilitates multiple scattering calculation for nanoparticles. Radiation forces are discussed in terms of scattering pressure and Lorentz force, hence Discrete Dipole Approximation (DDA) and classical Mie theory are employed in radiation force computation and electromagnetic random multiple scattering analysis. Electric momentum of dipoles is defined in the term of A-1 term method. The radiation forces on particles are accurately calculated with computer codes. Extracted results can be applied to conscious deviation of spherical nanoparticles in clean rooms or similar mediums. The effect of the incident wave parameters and the orientation of spherical profile and particles in the cluster are predicted through various simulations.

1. INTRODUCTION

The application of the nanotechnology in Medicine and Electronics has been introduced as a widespread technology in recent years. Splendid developments have been noticed in nanotechnology sciences, which leads to wide area of nano-electronics applications. Prominent features of the carbon nanotubes (CNT) in antenna design, application of nanoparticles in photonic crystals and usage of the CNTs to enhance the EM field absorption ratio in solar systems are in ongoing discussions in electronics engineering associations.

Movement of the nanoparticles in the presence of the EM radiation is a novel field of interest among scientific associations. Nanoparticles illuminated by an EM wave experience forces on them. Optical forces slightly deviate the nanoparticles. As a result, EM waves can be considered as a stimulant for nanoparticles.

Sunlight is an electromagnetic radiation originates from the Sun. Diffused radiation of the Sun is filtered by the atmosphere of the Earth, seen as daylight. Visible light already known as *White Light* includes specific electromagnetic spectrum between 380 to 780 nm, white light is a combination of seven different colors which can be detected by a prism. White light propagating in a prism can be decomposed to seven different EM waves.

Radiation forces exerted on particles with different size distributions have been discussed in several papers. Radiation pressure on fluffy dust particles in solar system has been calculated through multiple scatterings of particles by Kimura et al., and the dust particles and solar radiation pressure on them were investigated [1]. Radiation forces on a single particle in Ryleigh regime is also calculated by a laser beam illuminating the particle [2]. Micrometer-sized particles were also investigated in the presence of

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EM radiation, and the movement of the micrometer-sized particles illuminated by a laser beam was illustrated in photomicrographs [3].

Arbitrarily shaped particles were also considered in literature. Equilibrium of variously sized particles in the presence of the laser beam was discussed [4]. Either radiation forces on nanoparticles combined in a cluster or absolute value and direction of forces on nanoparticles are missing among papers in literature.

In this paper, reaction of nanoparticles to the white light is discussed in detail. Nanoparticles are considered to be dielectric spherical ones, randomly oriented in a cluster. Radiation pressure and Lorentz forces exerted on these spherical nanoparticles are calculated in terms of Discrete Dipole Approximation (DDA) and classical Mie theory, accurately. EM fields on each particle can be defined by multiple scattering analysis of mentioned clusters. Movement of nanoparticles due to the EM radiation is illustrated by different figures extracted by MATLAB software. The absolute value and direction of radiation forces are demonstrated in tables, respectively. Arbitrarily sized particles are illuminated by EM waves in visible light spectrum which models the radiation of the Sun. Simulations are done by a computational MATLAB code to demonstrate different orientations between nanoparticles.

2. THEORY

Electric dipoles can be approximated by particles much smaller than incident wavelength, where electromagnetic field on the particles is assumed to be constant. The incident wave induces a moment to tiny particles and assigns an electrical dipole on the particles, so they act as secondary radiation sources [5]. Radiation from these arbitrarily oriented dipoles composes the scattered field of the cluster. With the electrical momentum and EM field known on the particles, direction of deviation can be achieved through DDA.

2.1. Calculation of Dipole Polarizabilities

Positive and negative charges in a dipole tend to oscillate in the presence of EM radiation. The oscillation occurs by transposition of charges in dipole structure which leads to radiation. Tendency of electrical charges to transposition in a dipole is known as dipole polarization. Fig. 1 illustrates the polarized dipoles in the presence of applied electric field on them. Dipole polarization is dependent on material properties of particles and is different for various types of materials.

For spherical particles much smaller than incident wavelength, dipole polarization can be obtained by several methods. Claussius-Mossotti polarizability of the particle with relative permittivity of ε_s

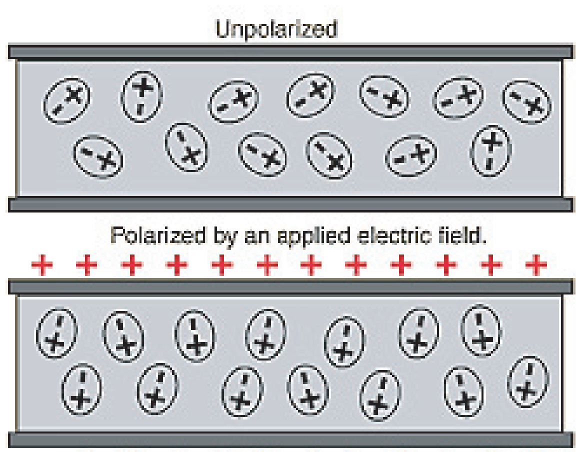


Figure 1. Polarized dipoles by an applied electric field.

confined in a finite volume with permittivity of ε_m can be obtained by the form below [6]:

$$\alpha = \frac{\alpha_{CM}}{1 - i\frac{2}{3}k^3\alpha_{CM}} \tag{1}$$

where:

$$\alpha_{CM} = \frac{a^3\left(\varepsilon_s - \varepsilon_m\right)}{\left(\varepsilon_s + 2\varepsilon_m\right)} \tag{2}$$

As seen in Eq. (2), polarizability is a matter of particle's radius and relative permittivity besides the medium permittivity. Another method to calculate the value of dipole polarization is based on the classical Mie Theory known as *A-1 Term Method*, and in this method, polarizability is dependent on the first Mie scattering coefficient [7]. Mie theory is the exact solution of scattering by an isotropic and homogenous sphere illuminated by plane wave. Scattering coefficients of Mie theory are calculated by the expressions below [8]:

$$\begin{aligned} a_n &= \frac{\mu_1\psi_n\left(\alpha\right)\psi_n'\left(\beta\right) - \mu_2 m\psi_n\left(\beta\right)\psi_n'\left(\alpha\right)}{\mu_1\xi_n\left(\alpha\right)\psi_n'\left(\beta\right) - \mu_2 m\psi_n\left(\beta\right)\xi_n'\left(\alpha\right)}, \\ b_n &= \frac{\mu_2 m\psi_n\left(\alpha\right)\psi_n'\left(\beta\right) - \mu_1\psi_n\left(\beta\right)\psi_n'\left(\alpha\right)}{\mu_2 m\xi_n\left(\alpha\right)\psi_n'\left(\beta\right) - \mu_1\psi_n\left(\beta\right)\xi_n'\left(\alpha\right)} \end{aligned} \tag{3}$$

In above expressions α, β stand for size parameters for free space and inside sphere. Also m stands for relative refractive index between particle (n_2) and propagation medium (n_1). Expressions in Eq. (3) are general ones in which magnetic properties of medium and particles are also considered. The Mie scattering coefficients are employed to expand scattered electric field in the terms of Vector Spherical Wave Functions (VSWF).

$$E^s = E_0\sum_{n=1}^{\infty}\sum_{m=-n}^{n} i\left[a_{mn}\bar{N}_{mn} + b_{mn}\bar{M}_{mn}\right] \tag{4}$$

VSWFs are calculated through Associated Legendre Functions to expand vector quantities in spherical coordinates [5].

$$\begin{aligned} \bar{M}_{mn} &= \left[\hat{e}_\theta i\pi_{mn}\left(\theta\right) - \hat{e}_\varphi\tau_{mn}\left(\theta\right)\right] z_n^{(l)}\left(\rho\right) \times \exp\left(im\varphi\right), \\ \bar{N}_{mn} &= \left\{\hat{e}_r n\left(n+1\right)P_n^m\left(\cos\theta\right)\frac{z_n^{(l)}\left(\rho\right)}{\rho}.+\left[\hat{e}_\theta\tau_{mn}\left(\theta\right) + \hat{e}_\varphi i\pi_{mn}\left(\theta\right)\right]\frac{\left[\rho z_n^{(l)}\left(\rho\right)\right]'}{\rho}\right\} \times \exp\left(im\varphi\right) \end{aligned} \tag{5}$$

Here $z_n^{(l)}$ is the proper form of the Bessel function due to expansion region. Associated Legendre functions follow these expressions:

$$\begin{aligned} \pi_{mn}\left(\theta\right) &= \frac{m}{\sin\theta}P_n^m\left(\cos\theta\right), \\ \tau_{mn}\left(\theta\right) &= \frac{d}{d\theta}P_n^m\left(\cos\theta\right), \\ P_n^m\left(x\right) &= \frac{\left(-1\right)^m}{2^n n!}\left(1-x^2\right)^{m/2}\frac{d^{n+m}}{dx^{n+m}}\left(x^2-1\right)^n \end{aligned} \tag{6}$$

A-1 term is dedicated to calculate dipole polarization through Mie scattering coefficients of individual sphere in the cluster.

$$\alpha_j = i\frac{3a_1}{2k^3} \tag{7}$$

Here, α_j is the polarization of jth dipole, and a_1 is the first Mie scattering coefficient defined in Eq. (3). The A-1 term method and the Mie scattering coefficients are employed to define polarization of spherical particles, which are considered as a single electric dipole.

2.2. Multiple Scattering

Suppose a cluster of L spheres which are arbitrarily oriented. Incident wave on cluster will be scattered through tiny spherical particles combined in the cluster. The total scattered field is the sum of the primary excitation wave and scattered field of each individual particle. Besides scattering by individual spheres, interaction between the particles should be considered. Incident wave illuminating jth sphere consists of excitation wave and scattered wave by any other particles in the desired cluster. Hence, to obtain the value of exerted force on particles, EM field on surface of the desired particle should have been calculated, previously. Discrete dipole approximation is employed to calculate EM field for confined dipoles in the cluster [9].

$$E_j = E_{inc,j} - \sum_{k \neq j} A_{jk} P_k \tag{8}$$

Interaction between particles in the cluster is about consideration of scattered field of a sphere as an incident wave for the other sphere. As seen in Eq. (8), A_{jk} is the expression for interaction involvement between jth and kth spheres. The first term in Eq. (8) is the primary excitation electric field, and the second term is consideration of scattered field by other particles on the jth sphere.

$$A_{jk} = \frac{\exp(ikr_{jk})}{r_{jk}} \left[k^2 \left(\hat{r}_{jk}\hat{r}_{jk} - I_3\right) + \frac{ikr_{jk} - 1}{r_{jk}^2} \left(3\hat{r}_{jk}\hat{r}_{jk} - I_3\right) \right] \tag{9}$$

where:

$$r_{jk} = |r_j - r_k|, \quad \hat{r}_{jk} = (r_j - r_k)/r_{jk} \tag{10}$$

Also P_k in (8) is the momentum of kth dipole follow below expression:

$$P_k = \alpha_k E_k \tag{11}$$

In the term of Eq. (8), electric field on the jth sphere will be achieved through confined cluster. Extinction cross section of the cluster is also calculated through Eqs. (8) and (11) [9]:

$$C_{ext} = \frac{4\pi k}{|E_0|^2} \sum_{j=1}^{N} \mathrm{Im}\left(E_{inc,j}^{*} \cdot P_j\right) \tag{12}$$

2.3. Definition of Scattering Pressure

Momentum transfer occurs as the oscillating dipole radiates secondary wave which changes the direction and amount of energy in EM wave. These changes lead to an exertion of force on particle known as *Scattering Force* [2].

$$P_{scat} = \hat{i}\left(\frac{\sqrt{\varepsilon_j}}{c}\right) C_{pr} \cdot I(r) \tag{13}$$

Scattering pressure or scattering force in the direction of incident wave ($\hat{i}$) defined in Eq. (13) is dependent on the total cross section (C_{pr}) and relative permittivity of the particle (ε_j), respectively. Parameters of C_{pr} and EM irradiance are defined by below expressions:

$$C_{pr} = \int_0^{2\pi} \int_0^{\pi} C_{sca} \sin\theta d\theta d\varphi, \quad I = \left\|\bar{E}_j \times \bar{H}_j^{*}\right\| \tag{14}$$

By substituting Eq. (14) in Eq. (13), scattering force on cluster can be accurately obtained.

2.4. Lorentz Force Calculation

Another exerted force on particles in the cluster is known as *Lorentz Force*. This kind of force is exerted on charges in EM field that can be obtained through dipole moment. Electric dipole consists of two opposite charges that are positioned in a small distance with each other. Opposite charges experience Lorentz force in EM field of incident wave [10].

$$\bar{F}_{Lorentz} = (\bar{p} \cdot \nabla)\, \bar{E} + \bar{p} \times \left(\nabla \times \bar{E}\right) + \frac{d}{dt}\left(\bar{p} \times \bar{B}\right) \tag{15}$$

Momentum in Eq. (15) is followed by the expression below:

$$\bar{p}_j = \alpha_j \bar{E}_j \tag{16}$$

Operating some mathematical techniques on Eq. (15), the expression will have a simpler form:

$$\bar{F} = \sum_i \bar{p}_i \nabla \bar{E}_i + \frac{d}{dt}\left(\bar{p} \times \bar{B}\right) \quad i = x, y, z \tag{17}$$

In expression above the term ∇E demonstrates relation between any component of the exerted force and gradient of electric field in all directions of Cartesian coordinate. The effect of magnetic flux (B) can be neglected compared to electric field due to smaller amplitude. In terms of Eqs. (13) and (17), all radiation forces exerted on nanoparticles can be accurately calculated. Next section demonstrates several simulations of nanoparticles illuminated by EM wave in various orientations.

3. SIMULATION

Several simulations for various particles with different electric parameters (size, relative permittivity, etc.) are performed through MATLAB software. Absolute value and direction of radiation forces composite of scattering pressure and Lorentz force are illustrated by figures and tables in later sections. Scattering pressure is calculated for the cluster of arbitrarily oriented spherical nanoparticles, but Lorentz force exerted on each individual nanoparticle is calculated in detail. Simulations are done by a Core i5 M460, 2.53 GHz CPU with 4 GB DDR3 RAM under Windows 7 operating system. Both discrete dipole approximation and the Mie theory are involved in the simulation algorithm, coded by MATLAB computational software. Different incident wave profiles through various orientations are the prominent features of simulation section.

3.1. Simulation No. 1

This simulation demonstrates a cluster of 7 arbitrarily oriented lossless dielectric spheres with the radius of $a = 80$ nm and relative permittivity of $\varepsilon_r = 3.5$ which are illuminated by an x-polarized ($\beta_p = 0°$) incident wave, with the wavelength of $\lambda = 600$ nm, propagating in $+z$ direction. Fig. 2 illustrates the orientation of spheres in the cluster. Radiation forces on this cluster will be demonstrated in detail, respectively. In this simulation, particles are far from each other compared to their size parameter. Notice that particles are magnified in size to achieve a better vision in the text.

Scattering pressure exerted on the cluster can be calculated through Eq. (13). Here scattering pressure vs. elevation angle (θ) is plotted in Fig. 3(a). As an example, the fixed azimuth angle ($\varphi = 0°$) is involved in calculations. Direction of exerted pressure as mentioned in Eq. (13) is parallel to incident wave on each particle which is shown in Fig. 3. So, electric field on each particle also shows the direction of radiation pressure according to Eq. (13). Direction of radiation pressure on particles in Fig. 3(b) is a unit vector which is normalized to the absolute value of exerted pressure. The amount of pressure is calculated for all the particles as a cluster which is shown in Fig. 3(a).

Exact value and direction of Lorentz force exerted on each particle is illustrated through Fig. 4 and Table 1. For each particle by its position in the coordinate system, Lorentz force vector is calculated in Table 1, and unit vector of direction is shown in Fig. 4.

Because of rotation angle and view of sight unit vectors can be considered in different values, but it should be noticed that these are unit vectors normalized by the absolute value of forces exerted on the particles. Table 1 demonstrates the vector of Lorentz force on each particle. Positions of the particles in Cartesian coordinates are illustrated in Table 1, respectively.

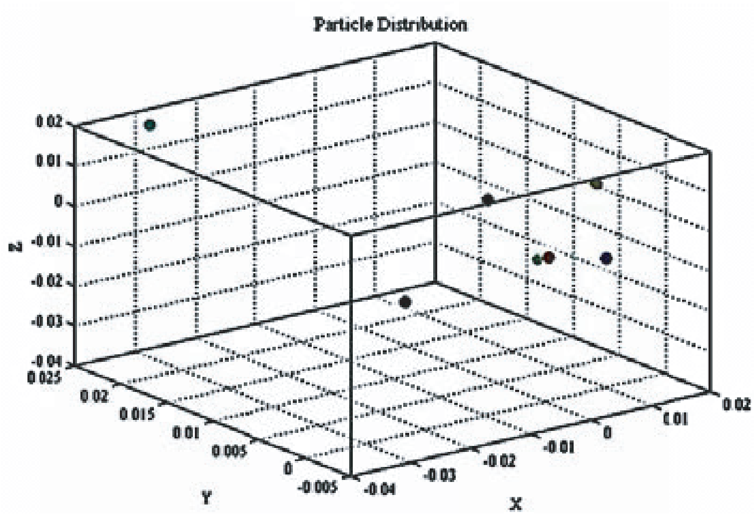
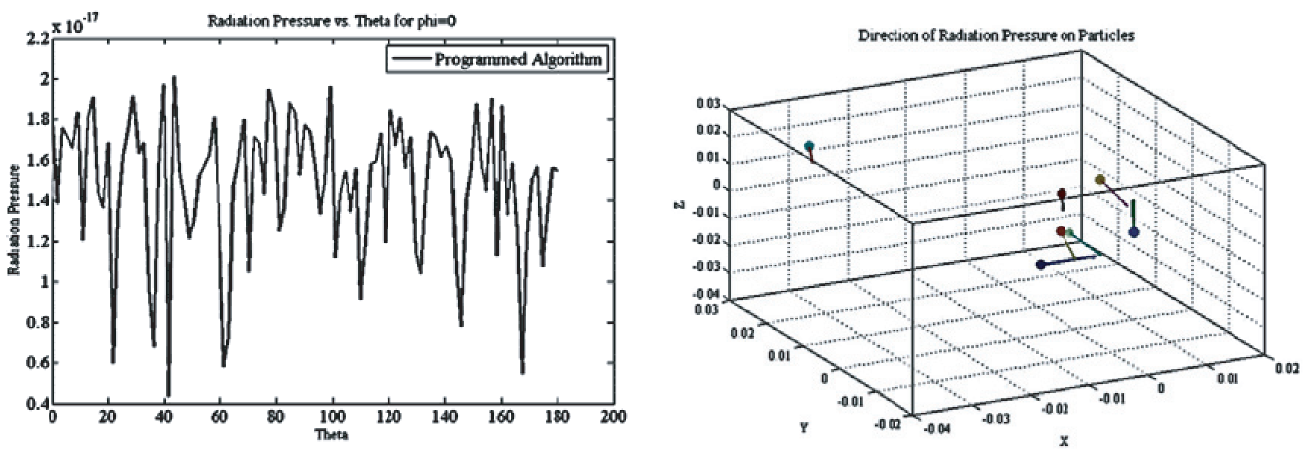


Figure 2. Particle distribution in simulation No. 1.



(a) (b)

Figure 3. Radiation pressure exerted on the cluster of spheres. (a) Amplitude. (b) Direction of pressure.

Table 1. Lorentz force vector definition.

No.	X (mm)	Y (mm)	Z (mm)	$F(N)$
1	-6.3	19.3	-34.9	$(-9.7\hat{x} + 3.2\hat{y})E - 23$
2	10.1	0	-7.8	$(-0.001\hat{x} + 5.1\hat{y} + 0.002\hat{z})E - 21$
3	-31.2	22.7	19.5	$(3\hat{x} + 4.1\hat{y} + 0.1\hat{z})E - 23$
4	-0.6	0.4	-4.8	$(1.18\hat{x} + 1.6\hat{y} - 0.003\hat{z})E - 21$
5	1.5	-4.6	18.2	$(-3.5\hat{x} - 1.1\hat{y} + 0.01\hat{z})E - 22$
6	-4.5	-3.3	0.6	$(0.6\hat{x} - 1.6\hat{y} - 4.7\hat{z})E - 23$
7	2.5	7.8	2.3	$(-7.6\hat{x} + 2.4\hat{y} + 0.1\hat{z})E - 22$

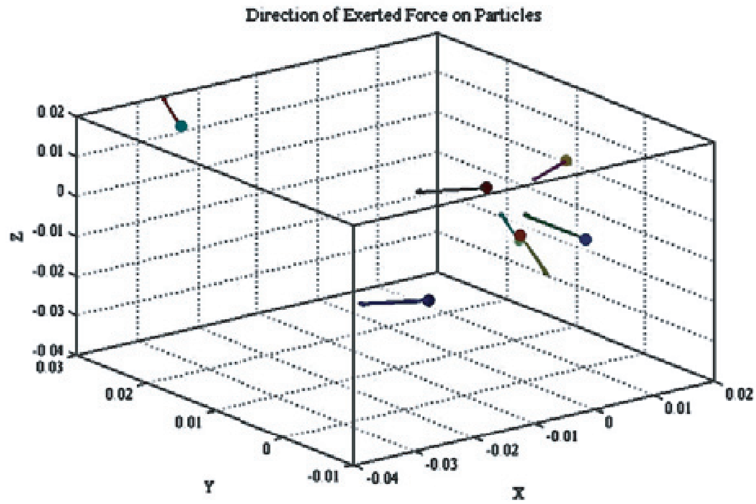


Figure 4. Direction of Lorentz force exerted on each particle.

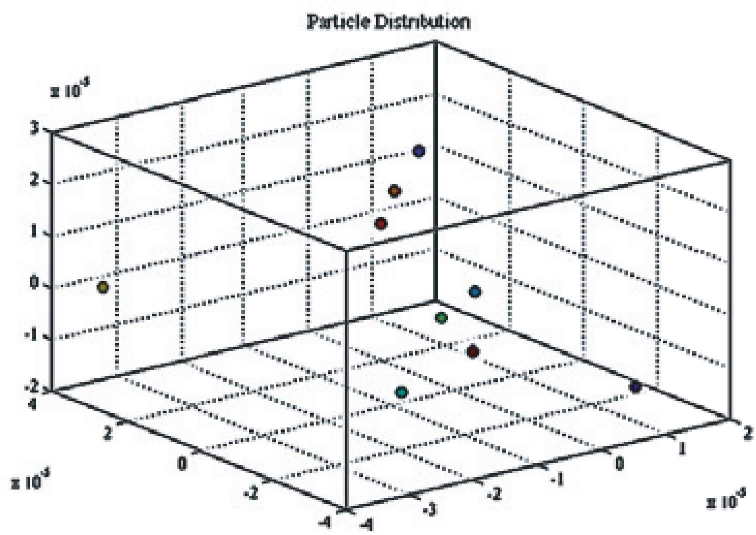


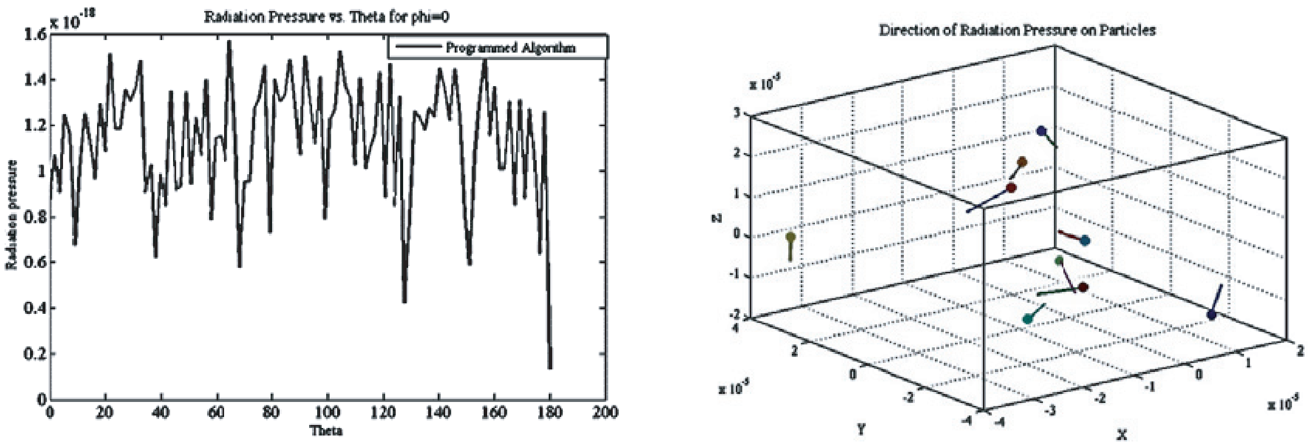
Figure 5. Particle distribution in simulation No. 2.

3.2. Simulation No. 2

This simulation demonstrates a cluster of 9 arbitrarily oriented lossy dielectric spheres with the radius of $a = 60\,\text{nm}$, relative permittivity of $\varepsilon_r' = 4$ and loss factor of $\varepsilon_r'' = 0.4$ which are lightened by x-polarized ($\beta_p = 0°$) incident wave, with the wavelength of $\lambda = 400\,\text{nm}$ propagating in $+z$ direction.

Similar to previous simulation, Fig. 5 also configures the orientation of particles in Cartesian coordinate system. Here, particles are much closer to each other, and inter-particle distance is comparable to the nanoparticles' size parameter. Again here particles are magnified to achieve a better vision. Radiation pressure on the mentioned cluster consists of 9 nanoparticles vs. elevation angle, demonstrated in Fig. 6(a). As mentioned before in this simulation particles are closer to each other which is obvious in Fig. 5's scales. Direction of illuminating electric field or similar direction of radiation pressure is illustrated in Fig. 6(b). Lorentz force calculations including value and direction of exertion are considered in this section through Fig. 7 and Table 2, similarly.

Results contain two important hints. The first one is demonstrated in Table 2 in which as particles



(a) (b)

Figure 6. Radiation pressure exerted on the cluster of spheres. (a) Amplitude. (b) Direction of pressure.

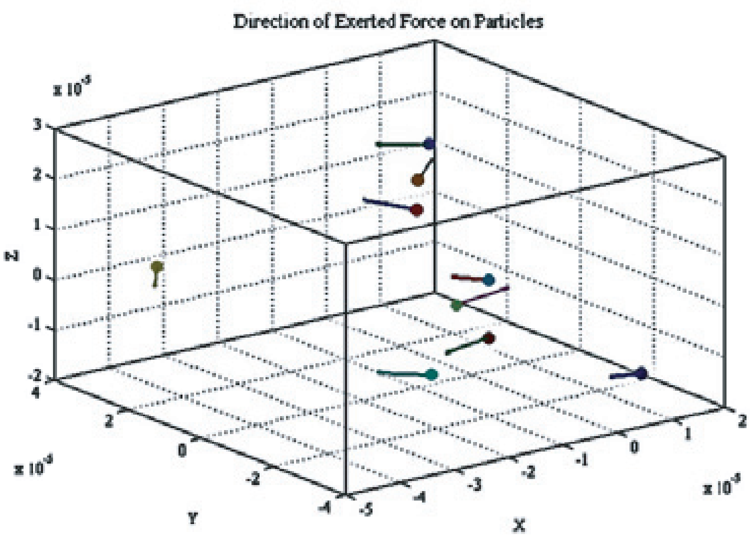


Figure 7. Direction of Lorentz force exerted on each particle.

get coarser, radiation pressure on them increases, and the second hint is about Lorentz force which has a bigger value as inter-particle distance decreases.

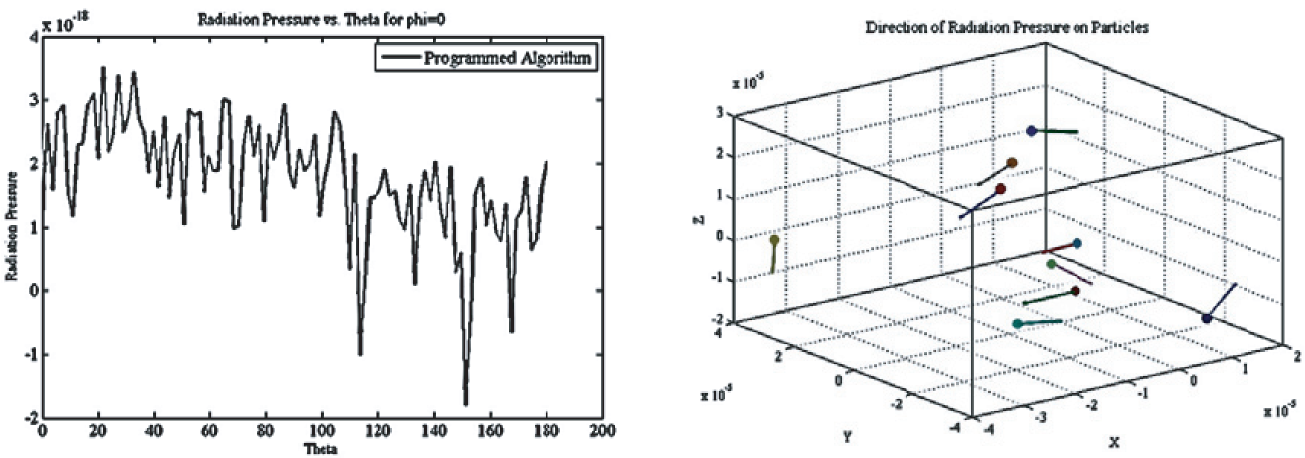
3.3. Simulation No. 3

Configuration and orientation of particles in this simulation are totally same as previous one. Cluster contains 9 spheres illustrated in Fig. 5. Radius and relative permittivity are also in the same manner. The purpose in this simulation is the investigation of polarization effect. Incident wave profile is a linearly polarized wave by polarization angle of ($\beta_p = 60°$). The change in polarization angle affects the parameters calculated in previous sections. Fig. 8(a) illustrates the radiation pressure on the cluster through elevation angle (θ) in a new incident profile.

Polarization change also influences the direction of electric field on each field which directly defines the radiation pressure's direction. Different polarization profiles such as the elliptic polarization and circular polarization can be applied to calculations, in which all investigations should be done for new profile [11]. Direction of radiation without loss of generality in all cases is in $+z$ direction. The amplitude

Table 2. Lorentz force vector definition.

No.	X (μm)	Y (μm)	Z (μm)	$F(N)$
1	10.1	−31.2	−13	$(-1.5\hat{x} - 0.7\hat{y} + 0.4\hat{z})E - 19$
2	7.4	22.8	17.5	$(-8.5\hat{x} + 1.4\hat{y} + 1.7\hat{z})E - 19$
3	3.1	0	−1.8	$(-0.3\hat{x} + 3.2\hat{y} - 0.5\hat{z})E - 18$
4	−14.3	−10.4	−13.3	$(-0.8\hat{x} + 1.2\hat{y} - 0.07\hat{z})E - 19$
5	2.6	7.9	−8.9	$(9.7\hat{x} - 1.3\hat{y} + 1.6\hat{z})E - 19$
6	−38.9	28.3	3.3	$(-\hat{x} - 1.4\hat{y} - 0.1\hat{z})E - 19$
7	−6.6	4.8	19	$(1.1\hat{x} + \hat{y} + 0.13\hat{z})E - 18$
8	−19.9	−14.5	22	$(-4\hat{x} + 6.6\hat{y} + 0.7\hat{z})E - 19$
9	0.98	−3	−12	$(-1.8\hat{x} - 0.3\hat{y} + 0.06\hat{z})E - 18$



(a) (b)

Figure 8. Radiation pressure exerted on the cluster of spheres in secondary incident wave profile. (a) Amplitude. (b) Direction of pressure.

Table 3. Lorentz force vector definition.

No.	X (μm)	Y (μm)	Z (μm)	$F(N)$
1	10.1	−31.2	−13	$(4.2\hat{x} + 1.2\hat{y} + 0.2\hat{z})E - 19$
2	7.4	22.8	17.5	$(-1.7\hat{x} + 0.5\hat{y} - 0.02\hat{z})E - 18$
3	3.1	0	−1.8	$(-4.1\hat{x} + 4.3\hat{y} - 7\hat{z})E - 18$
4	−14.3	−10.4	−13.3	$(1.3\hat{x} - 2.3\hat{y} + 0.4\hat{z})E - 19$
5	2.6	7.9	−8.9	$(-3.6\hat{x} + 1.7\hat{y} + 0.5\hat{z})E - 19$
6	−38.9	28.3	3.3	$(-5\hat{x} - 6.8\hat{y} - 1.3\hat{z})E - 20$
7	−6.6	4.8	19	$(2.3\hat{x} + 2.3\hat{y} + 0.2\hat{z})E - 18$
8	−19.9	−14.5	22	$(-0.8\hat{x} + 1.1\hat{y} - 0.3\hat{z})E - 18$
9	0.98	−3	−12	$(-7\hat{x} - \hat{y} + 0.3\hat{z})E - 18$

of incident wave (E_0) is considered to be normalized one, as predicted amplitude change directly affects the values of radiation pressure and Lorentz force. The Lorentz force vector and direction of exertion are presented in next sections and illustrated by Fig. 9 and Table 3.

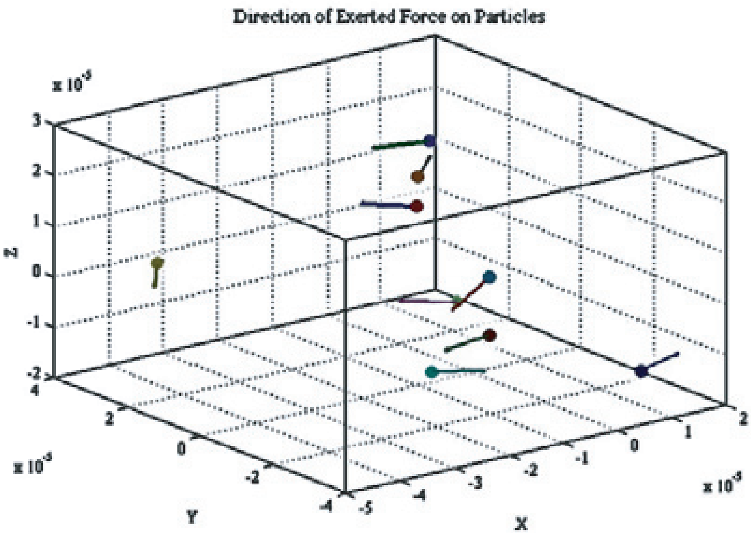


Figure 9. Direction of Lorentz force exerted on each particle.

4. CONCLUSION

Nanoparticles in the presence of the EM radiation are the main discussion in this paper. Different types of radiation forces such as scattering pressure and Lorentz force exerted on the particles are investigated through multi-particle scattering methods. Discrete dipole approximation and classical Mie theory are employed to calculate electric field on each individual particle confined in a cluster. In terms of DDA, particles with small size compared to incident wavelength are considered as electric dipoles. By the application of multiple scattering and A-1 term method, electric field on each particle and electric momentum of dipoles are accurately calculated. Driven MATLAB code for calculation of the radiation forces is simulated through several conditions with various orientations for particles in the cluster. Radiation pressure on the whole cluster and Lorentz force exerted on each particle are parameters simulated by computational MATLAB software. Through this paper's discussion, it can be concluded that nanoparticles experience a radiation force in the presence of the EM radiation, hence visible light spectrum has been considered, so nanometer-sized particles in the solar system also experience these radiation forces in the Earth's atmosphere, and by neglecting the other exertion forces such as gravity, direction of motion is demonstrated through various simulations in this paper.

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