

**AC 2008-2783: AN INTERACTIVE VIRTUAL REALITY SIMULATION FOR
NANOPARTICLE MANIPULATION AND NANO-ASSEMBLY USING OPTICAL
TWEEZERS**

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An Interactive Virtual Reality Simulation for Nanoparticle Manipulation for Nano-assembly using Optical Tweezers

1. Abstract

Nanotechnology and nanodevices is believed to be one of the most promising steps that science is taking to the future. This paper proposes virtual reality (VR) as a tool to simulate nanoparticle-manipulation using optical tweezers towards achieving nano- assembly for effectively handle issues such as difficulty in viewing, perceiving and controlling the nano-scale objects. The nano-simulation is modeled, using virtual reality, displaying all the forces acting on nanoparticle during the manipulation. The simulation is developed for particles that belong to Rayleigh region and, represents interactions of OT (a laser beam) with the nanoparticle. The laser beam aimed on to the nanoparticle traps the particle by applying optical forces. The trapped particle is then moved by moving the laser beam. The proposed VR based simulation tool with it capabilities 1 can be easily extended and used for creating and open system framework by connecting it to a real OT setup to control nanoparticles manipulation. In addition, a feedback system can be build to increase of precision of movement.

Keywords: Virtual Reality, Optical Tweezers

2. Introduction

Scanning Tunneling Microscopy (STM) [1], Atomic Force Microscopy (AFM) [2] and Optical Tweezers (OT) are some techniques used for nanoparticle manipulation. AFM is a contact method for nanoparticle manipulation. This method has limitations such as wear of the tool tip and particle getting stuck to the tip of the AFM probe making it difficult to release the particle at difficult at desired location. While STM is a non-contact method, it can work only in vacuum conditions and is restricted to conducting and semi-conducting materials. The above discussed drawbacks along with incapability to manipulate particle in X, Y and Z directions make AFM and STM less desirable for effective nanoparticle manipulation. The disadvantages can be overcome by using OT as a manipulation technique. OT is a non contact method which can be used to grab, move and release particles in three dimensional (3-D) space. In addition, the magnitude of forces in OT is very small of the magnitude of *pico* and *nano* Newton which can make OT the most desirable method for manipulating nanoparticles.

The transformation of OT from single particle manipulation [3, 4] to several particle manipulations towards nanoassembly has progressed significantly. OT is being experimented with several techniques such as Chemical assembly [5] and Holographic Optical Tweezers [6] to achieve nanoassembly. The applications of OT range from bio-medical sciences to chemistry to technology.

The size of the nanoparticles and their force magnitudes make it difficult to visualize the manipulation process in real time. The ability of VR to visualize real time process and control it by acting as an interface between user and real world make it the most desirable method to interact with nano-world.

2.1 Physics of OT

OT consists of a laser beam focused on the nanoparticle, to trap or grab the nanoparticle and place it at a required point or destination. Laser beam has photons which carry momentum. When the beam hits the particle, the photons tend to lose their momentum which is converted as force (radiation force) according to Law of Conservation of Momentum. The particle is trapped in the resultant direction of the force obtained from all the photons of the beam. [7, 8]. This trapped particle is then moved or manipulated by moving the laser beam.

To manipulate the particle, it is important to know all the forces acting on the particle before, during and after the manipulation. Depending on the size of the particle, different theories are proposed to calibrate forces on the particle. Particles of size less than wavelength of light (laser beam) are categorized under Rayleigh Regime and those more than wavelength of light, under Mie Regime. For particles whose size is equal to wavelength of light an intermittent theory is used. OT is specifically helpful in handling small particles or Rayleigh particles. This paper discusses work done on manipulation of Rayleigh particles using OT.

As described earlier, the laser beam imparts force upon hitting the particle. This force is split into two components. When light reaches the particle, it polarizes the particle and due to this the particle is pulled towards the highest intensity of the beam resulting in one of the force component called gradient force. This force makes particle instable. The instability is eliminated by another force component called scattering force. This force is due to photons in light which tend to apply forces (due to momentum transfer) on the dielectric particle along the propagating path. Scattering force depends on momentum transfer of photons which in turn depends on angle of incidence of photons on the particle. The angle of incidence can be changed by varying refractive index of the medium surrounding particles. Thus, it can be understood that scattering force depends on refractive index of surrounding medium. Gradient force on the other hand depends on laser beam intensity as intensity is proportional to polarization.

Figure 1 shows two beams (PQRS, IJKL), hitting a particle with focus, (F), before (Figure 1a) and after (Figure 1b) the particle [9]. The momentum transfer, due to change in propagation direction, for incident ray IJ and PQ is shown as M_1M_2 and M_3M_4 . The resultant of the moments $M_1 M_5$ or M_3M_5 is the direction in which the gradient force acts.

Though optical forces are dominant while trapping the particle, the particle being on substrate, experiences various forces which have to be accounted for while manipulating the particle. In the

next step, methodology, different forces and their equations are analyzed and programmed into VR software to run the simulation.

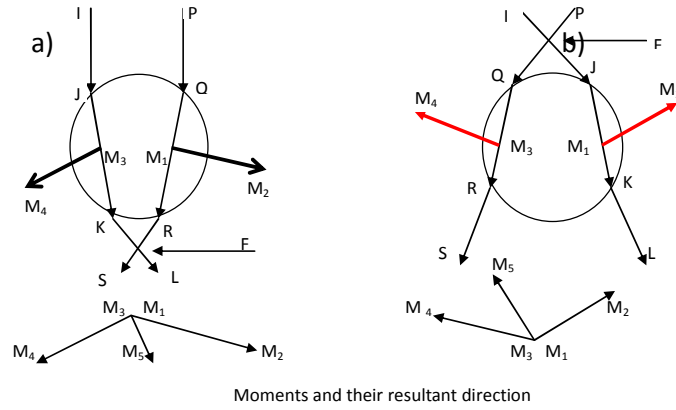


Figure 1 Physics of OT

3. Methodology

Once theory is determined, different forces and their impact on nanoparticle is studied and analyzed. Methodology involves developing force equations and programming them into VR software. A mathematical system involving force equations is developed. The equations are solved and fed into VR simulation model. The equations are triggered and the force is applied on nanoparticle thereby achieving the manipulation task in VR simulation model. The forces can be categorized as optical and non-optical forces which are explained in the following sections

3.1 Forces acting on the particle

3.1.1 Optical forces

For the particle to be stable in the trap it is important that the gradient force on the particle should be significantly more than the scattering force. For a single beam trap on a particle in Rayleigh regime, gradient and scattering force are given by equations 1 and 2[10]

Gradient force can be represented by,

$$F_{grad,z(r)} = -\hat{z} \frac{2\pi n_2 a^3}{c} \left(\frac{m^2 - 1}{m^2 + 2} \right) \left(\frac{8(\hat{z} / (kw_0))^2}{1 + (2\hat{z})^2} \right) \left[1 - \frac{2(\tilde{x}^2 + \tilde{y}^2)}{1 + (2\hat{z})^2} \right] \left(\frac{2P}{\pi w_0^2} \right) \quad (1)$$

$$X \frac{1}{1 + (2\hat{z})^2} \exp \left[-\frac{2(\tilde{x}^2 + \tilde{y}^2)}{1 + (2\hat{z})^2} \right]$$

Scattering force is give by,

$$F_{scat(r)} = \hat{z} \frac{n_2}{c} \left(\frac{m^2 - 1}{m^2 + 2} \right) \left(\frac{8(ka)^4 a^2}{3} \right) \left(\frac{2P}{\pi w_0^2} \right) X \frac{1}{1 + (2\hat{z})^2} \exp \left[-\frac{2(\tilde{x}^2 + \tilde{y}^2)}{1 + (2\hat{z})^2} \right] \quad (2)$$

Where,

‘ \hat{z} ’ - is unit vector, $P = \left(\frac{\pi w_0 n_2 \varepsilon_0 c E_0^2}{4} \right)$ is the laser beam power (Watt),

‘ ε_0 ’ dielectric constant of the medium, E_0 amplitude of intensity (V/m), ‘ n_2 ’ refractive index of the surrounding media, $(\tilde{x}, \tilde{y}, \tilde{z}) = \left(\frac{x}{w_0}, \frac{y}{w_0}, \frac{z}{kw_0^2} \right)$ represent the normalized spatial coordinates,

$m = \left(\frac{n_1}{n_2} \right)$ is the relative refractive index of the particle, $k = \left(\frac{2\pi}{\lambda} \right)$ represents the wave number of laser beam, ‘ a ’ particle radius in nm, ‘ w_0 ’ beam waist.

3.1.2 Other forces acting on the particle

Since the particles are placed on substrate, forces between particle and substrate have to be considered. Due to small size of particles, contribution of intermolecular forces towards the total force is significant. The intermolecular forces between substrate and particle are the capillary force, Van der Waals force and the electrostatic force.

Further, if the particles are suspended in liquids then Brownian motion should also be considered. The inclusion of Brownian motion gives scope for our VR model to be applied for different possible cases of particle manipulation.

3.1.2.1 Capillary Force

Capillary force is the force between two particles. If particles are placed on fluidic medium then the force equation between particle and fluid can be written as Equation (3) [11]

$$F_c = 2\pi a \gamma \quad (3)$$

‘ γ ’ (gamma) is the surface tension of the substrate and ‘ a ’ being radius of the particle.

3.1.2.2 Van der Waals Force

Vander Waals forces are weak attractive intermolecular forces. These forces arise when two particles come close to each other. These forces can be calibrated using Lenard-Jones equation (4) [11].

$$F_c = \left(\frac{A}{6} \right) \left(\frac{s}{h^2} \right) \left(\frac{z}{4h^2} - 1 \right) \quad (4)$$

Where

'h' is the distance between two particles, 'A' the Hamacker constant, 'Z' the separation of lowest energy between the two particles that are under Van der Waals forces, 's' Derajaguin geometrical constant which is related to mutual curvature between particles in contact.

3.1.2.3 Electrostatic Force

Since the sphere is electrically charged, electrostatic forces, which are between charged sphere and uncharged planes, have to be considered. These forces can be calibrated from the equation (5) [11]

$$F_E = \left(\frac{\pi}{\epsilon_0} \right) \left(\frac{\epsilon - 1}{\epsilon + 1} \right) \sigma^2 a^2 \quad (5)$$

Where

' σ ' is the charge surface density, ' ϵ ' and ' ϵ_0 ' are the permittivity values in vacuum and dielectric substrate respectively and 'a' is the radius of the particle.

3.1.2.4 Gravitational force

The effect of gravity on the particle is almost negligible in all operating conditions. The expression to calculate gravitation force is (6) [11]

$$F = \left(\frac{4}{3} \right) \pi \rho g a^3 \quad (6)$$

Where 'g' is the gravitational constant equal to 10 ms^{-2} ,

' ρ ' is the density of the particle in kgm^{-3} and 'a' is the radius of the particle.

Though the effect of gravitational force is negligible for particles nanometer in size, it is in the interest of considering all the possible forces on the particle that this force has also been included in the analysis.

3.1.2.5 Brownian force

If the particles are suspended in fluidic medium, they experience Brownian force due to extreme small size. Brownian force is due to continuous collision of the nanoparticles with the liquid particles. This moves the particles haphazardly in the fluidic medium. This motion is called Brownian motion and can be modeled by Fokker plank equation. The Brownian equation can be given as Equitation (7) [12].

$$U(z) = U_0 \exp \left\{ \left(\frac{2\alpha\pi n}{ck_B T} \right) I(0) \exp \left(\frac{-z}{\delta} \right) \right\} \quad (7)$$

Where

' α ' is the polarizability, 'c' is velocity of sound, ' K_b ' is Boltzman constant, 'T' is temperature, 'I' is intensity of laser, 'z' is distance of particle from focus of laser, ' δ ' is decay length of laser beam, ' $U(z)$ ' is density at a distance of 'z', ' U_0 ' is the initial density of particles.

3.2 VR simulation model

The VR simulation includes a laser beam (OT) and a nanoparticle placed on substrate as a system. The force equations derived are modeled into VR software so that when the beam approaches the particle, force equations are triggered to apply force on the nanoparticle. The forces acting on the particle are shown as vectors. The vectors are scaled up or down for better visualization purpose. The magnitude of forces can be determined by sending the values to a file at target location. Thus, a working VR simulation is with display of forces on particle while being manipulated.

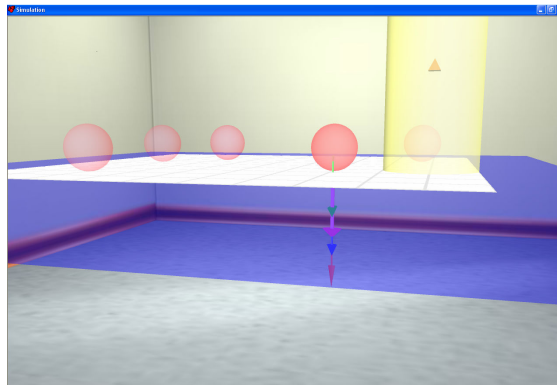


Figure 2 VR simulation of OT process

Figure2 shows the VR simulation model of OT. The particles (orange spheres) at various positions are placed on a table (blue plate) with substrate (white grid plate). The laser beam (OT) is represented as a yellow semi-transparent cylindrical object. The focus of the laser beam is represented as a dark spot (pyramid) inside the laser beam. Different colors for vectors have been used in order to represent different forces. The force vectors can be seen having different lengths and thicknesses. It is to be remembered that there is no universal scaling factor followed for all vectors. This is because such method would result in too small vectors for forces having small magnitude and too big vectors for higher force magnitudes. This would make it difficult for human to view all vectors within the confined region around the sphere. To overcome this, each vector is scaled only graphically without changing the magnitude value in the simulation. The model should be considered as one that focuses on particle manipulation rather than one which has complete OT setup with experimental apparatus.

4. Results

To validate the developed mathematical model, we compared graphically our model with the experimental results [11]. The graphs matched closely to the experimental results.

The following assumptions made while developing the results.

The beam used on particle is a moderately focused zero order Gaussian beam (with Poynting vector $s = 0.012$ satisfying the condition for a zero order beam) having wavelength (λ) of $0.5145 \mu\text{m}$, beam waist (w_0) $5 \mu\text{m}$ and power of beam being 0.1mW . The relative refractive index 'm' is 1.191 where 'm' is ratio of refractive index of polystyrene sphere to refractive index of water.

Figure 3a is graph for 5nm particle with gradient force (in Newton) against the normalized spatial longitudinal distance between the center of the particle to the laser beam focus while 3b is plotted with same X axis while replacing Y axis with scattering force.

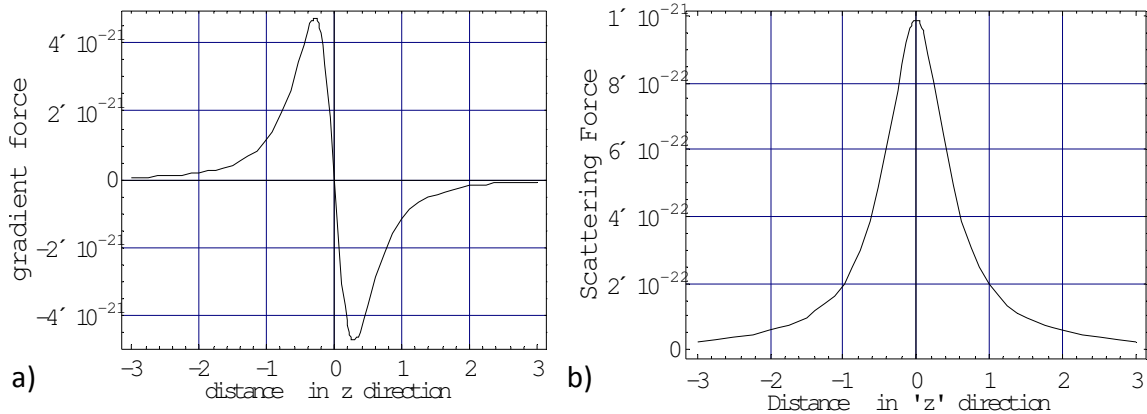


Figure 3 Gradient and Scattering forces for 5nm particle size

In Figure 3a, the gradient force has maximum magnitude near the focus of the laser beam. Though the gradient force in Figure 3a attains a negative value this change of sign should be attributed to the change in direction of gradient force but not to the magnitude of the force vector. As shown in Figure 3a and 3b at the focus point, the magnitude for gradient force is zero while for scattering force it is maximum. Due to this, the particle is pushed away from the focus along the direction of propagation of laser beam. As the distance between the focus and particle increases the gradient force dominates scattering force, holding back the forward moving particle. Thus for effective trapping, gradient force should dominate scattering force.

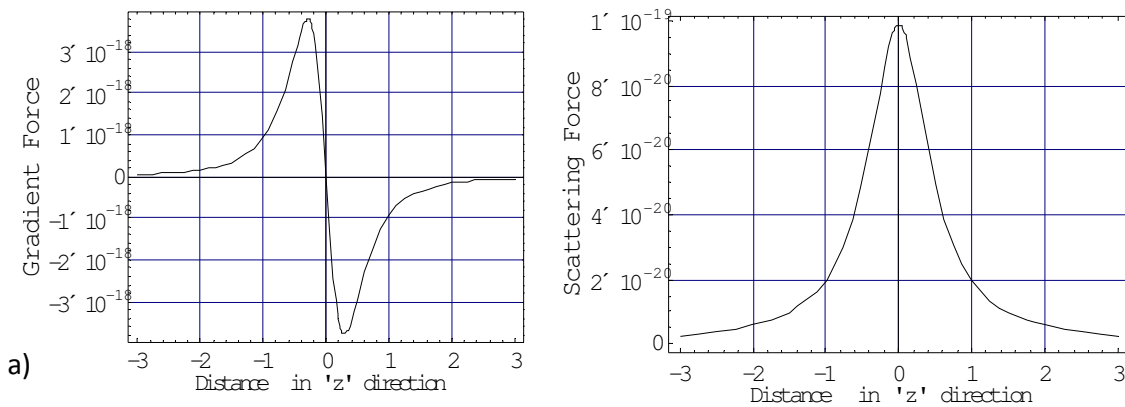


Figure 4 Gradient and scattering forces for 10nm particle

Figure 4a and 4b are plotted with X and Y axis same as those represented for Figure 3a and 3b respectively. Figure4 follows same pattern as observed for Figure3 except for the change in magnitude of gradient and scattering force which is due to change in the particle size.

It can be inferred from the graphs that the magnitude of the forces for particle of 5nm is much lesser than those for 10nm particle. Thus, as the particle size decreases the magnitude of force decreases drastically thereby making it more difficult to trap the particle.

4.1 OT simulation

The VR simulation model developed is shown below with an explanation of each stage of manipulation. The pictures show four different stages: resting stage, trapping stage, manipulating stage and release stage.

4.1.1 Resting stage

In the below figure (Figure 5a), the particle is free with no laser beam on it. The task is to move sphere from one point towards a structure (closed circle in this figure). This simple task can be repeated or extended to several particles to achieve nanoassembly process. The forces in the resting stage are forces between particle and substrate namely Brownian (orange vector), capillary (blue vector), gravitational (green vector) and electrostatic force (pink vector).

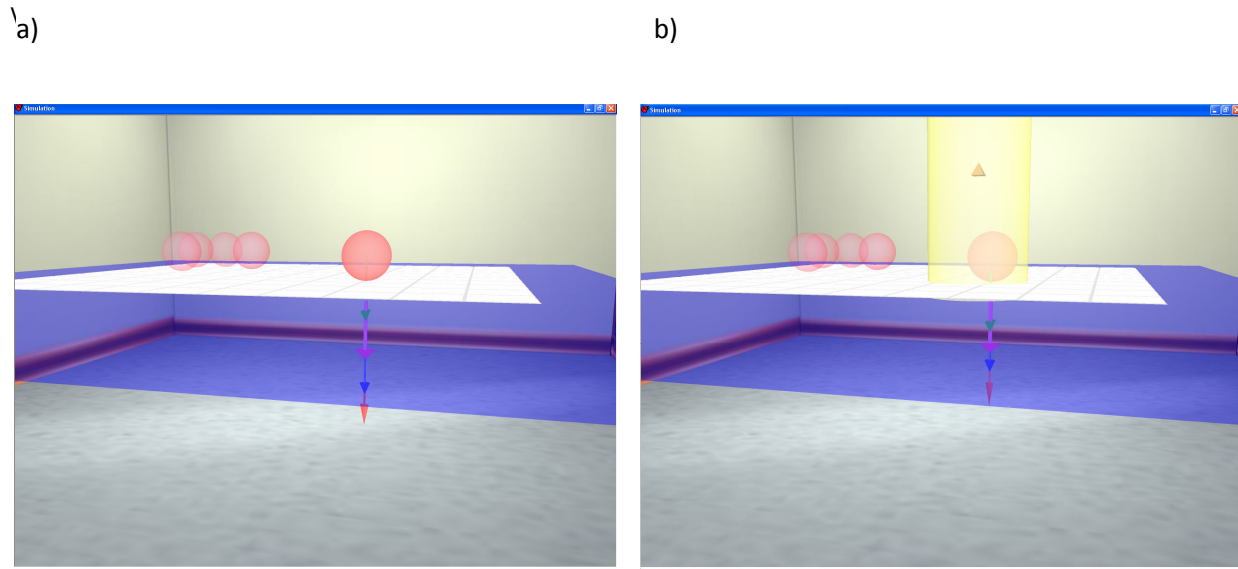


Figure 5 a) particles resting on substrate before laser beam is applied
b) Particle position before being trapped by OT

4.1.2 Trapping Stage

In the trapping stage (Figure 5b) the particle is trapped. The above figure shows laser beam activated on to resting nanoparticle. The optical force equations are triggered and are applied onto particle trapping it towards the focus of the laser beam.

Figure 6a. shows what happens after the forces are applied on to the particle. As the forces are applied the particle is lifted from the substrate. As the distance between particle and substrate increases, the forces the intermolecular forces between particle and substrate decrease. The forces that hold the particle are scattering force, gradient force and the gravitational force. The gradient force points towards the focus (pyramid in the laser beam) while the scattering force points downwards along the direction of propagation of light. Among the three vectors, the gradient vector exceeds in magnitude. To indicate this, the thickness of gradient vector is more than those of other vectors. The particle is lifted towards focus until the resultant of all forces becomes zero.

a)

b)

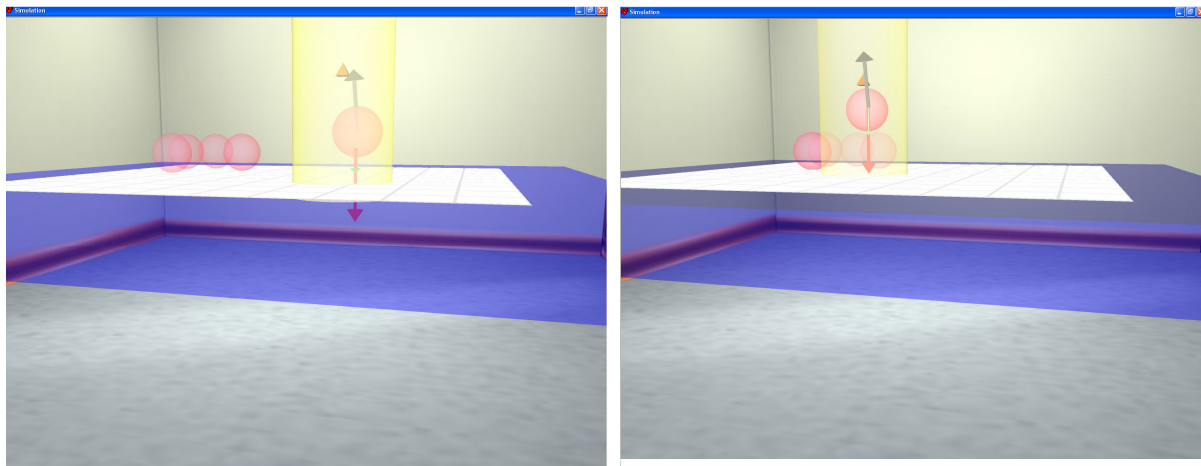


Figure 6 Nanoparticle movement

a) Particle lifted up after applying optical forces, b) Particle trapped and moved to destination

4.1.3 Manipulation Stage

Once the particle is lifted it is then transported to the destination position. In the Figure 6b particle is trapped completely and moved from the current position to the destination position. Presence of gradient force (grey vector) vector, scattering force (red vector) vector and gravitational force vector vectors implies that these forces are active. During the manipulation stage the particle is stable. As discussed in graphs, the particle is always instable at focus. Either the particle is trapped above or below the focus which can be seen in the below figure.

4.1.4 Release stage

Figure 7 shows the release stage. Once the particle reached its destination position the laser beam is turned off and the particle is released from the laser beam. As the particle comes close to substrate the intermolecular forces arise which can be seen in the below figure in the forms vectors pointing downward direction.

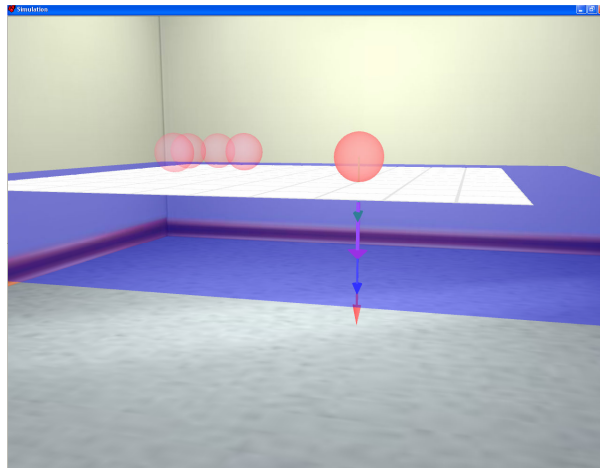


Figure 7 Particle released from trap to the target position

5. Conclusions

A VR simulation system for nanoparticles manipulation has been developed. The simulation is unique in terms representation and calculation of dynamic nature of forces, vector representation of forces and control over the manipulation process. A mathematical model was developed to solve force equations and was graphically compared with experimental results to validate the model. The results matched closely making our mathematical model with force equations represent forces in real OT setup. The results from mathematical model that includes force equations is then fed into VR simulation capable to apply forces in real time. The developed simulation can be used for manipulation tasks of various particle sizes within the Rayleigh regime. The VR simulation model with vector representation of forces and magnitude can provide user with a tool for easy way to perform nanoparticle manipulation. It opens the nanomanipulation field even to an ordinary, allowing to easy adoption and wider application development towards advanced nanomanufacturing.

Connecting the simulation to the OT setup is the next step we would like to proceed in our work. VR simulation will act as an interface for OT setup. The user would move the particle in the simulation which will be transferred to the OT through a control system. Once the particle is moved, the actual destination position of the particle can be sent back from OT setup through feedback. This would give user an idea of actual position of particle and user can make corrections in the simulation to achieve desired position for the nanoparticle. Further a feedback mechanism that will send back the actual position of the nanoparticles will improve the precision.

6. References

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