Optical Forces and Torques Acting on Non-Spherical Metallic Particles

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Summary

Metallic nanoparticles are nowadays used in various areas of biology chemistry or physics, e.g. they are used as a heat source causing hybridization of DNA or probes for surface enhanced Raman spectroscopy. Laser manipulation with such metal nanoparticles enables their precise delivery to the targets and their confinement for a given time. A single tightly focused laser beam – **optical tweezers** – was also employed to three-dimensional trapping of gold and silver nanoparticles with diameters between 20 to 250 nm [1, 2]. However, theoretical models assuming the spherical shape of a nanoparticle predict spatial confinement only for particles with diameter lower than 100 nm.

We show that the shape of nanoparticles is a key parameter that enables their trapping even by the low NA objective optical tweezers. Especially larger flat particles tend to reorient themselves perpendicularly to the beam polarization which strongly decreases their scattering and enables the optical trapping [3, 4].

Golden Nanoparticles

Noble metals form variously shaped nanoparticles (NPs) during their growth because they crystallize in a face-centered cubic lattice. Various shapes may be prepared by the different chemical conditions of their growth, i.e. sphere, cube, cuboctahedron, octahedron, decahedron or various plates [5]. Typically mixture of particles is prepared. We studied golden NPs having nominal diameters 50 nm up to 250 nm produced by the British Biocell company. Figure 1 shows Scanning Electron Microscopy image of particles having nominal diameter 100 nm and its right part shows various particle shapes present. Note that no spherical particle is present.

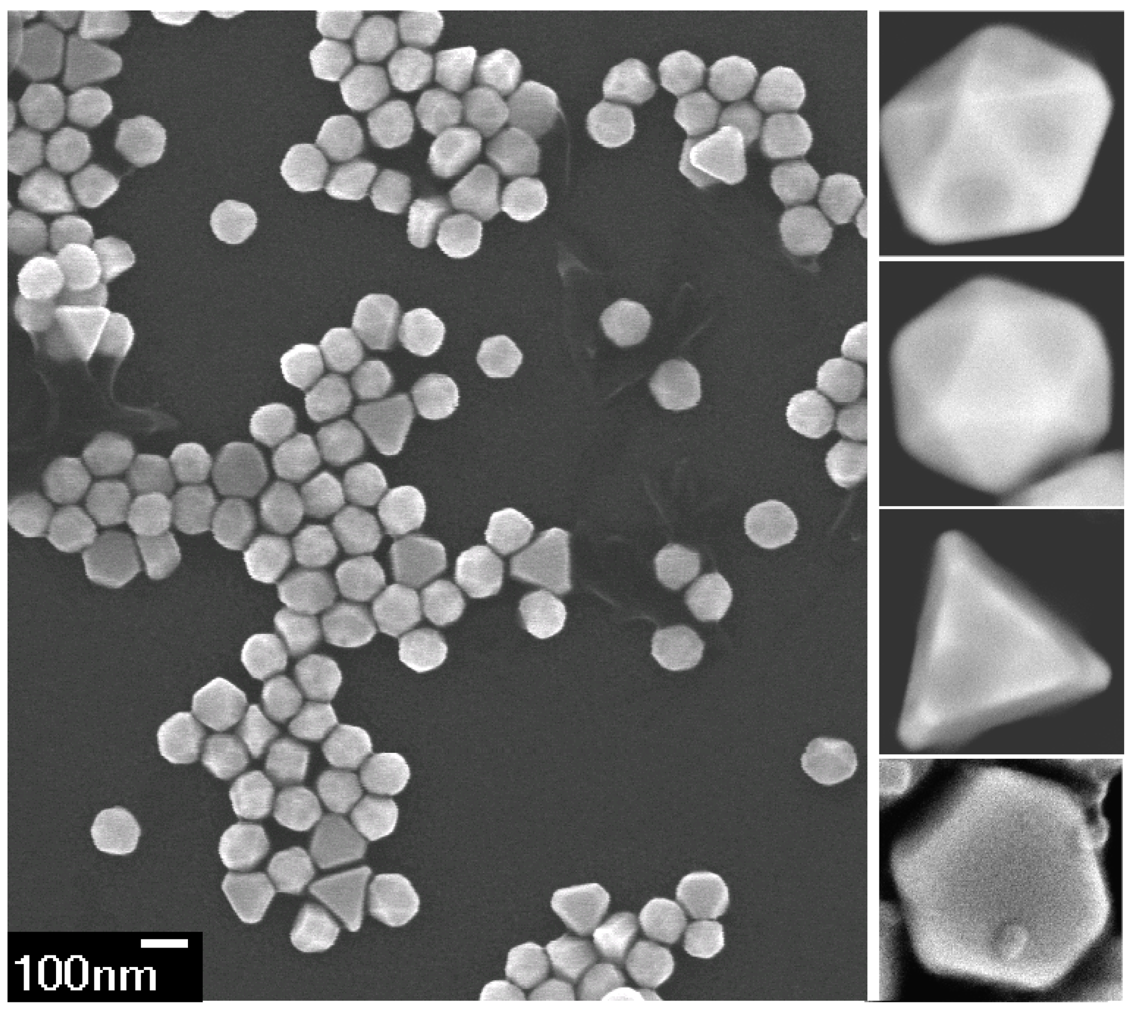

Figure 1: *Gold NPs (British Biocell, nominal diameter 100 nm) observed via scanning electron microscope (Magelan, FEI). Right-hand column shows detailed images of various particle shapes: decahedral bi-pyramid, icosahedron, triangular and hexagonal plates.*

Optical tweezers

Optical tweezers (originally called "single-beam gradient force trap") are scientific instruments that use a highly focused laser beam to provide an attractive or repulsive force (typically on the order of piconewtons) to physically hold and move microscopic dielectric objects. Small objects are pushed towards the places of high electromagnetic field intensity due to the "gradient force" and accelerated along the field propagation direction by the "scattering force," see figure 2a. If the resulting force changes sign from positive to negative stable trapping position occurs. This condition is hard to meet namely for metallic absorbing particles.

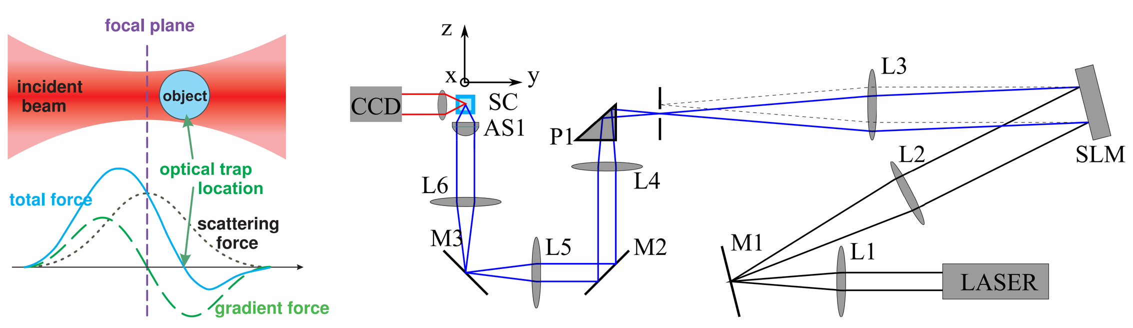

Figure 2: *(a) "Gradient" and "scattering" forces occuring near focal plane of tightly focused laser beam. (b) Experimental setup, for details see [6].*

We used a low numerical aperture optical tweezers (NA ~ 0.37-0.17, corresponding beam waist radii $w_0 = 0.91 - 1.7\,\mu\mathrm{m}$, λvac = 1064 nm), see figure 2a, to manipulate and trap these golden NPs.

Computational Methods

The calculation of optical force $\mathbf{F}$ and torque $\mathbf{T}$ is based on integrating Maxwell stress tensor $\hat{T}$ over a surface enclosing the studied object as follows

$$\langle \mathbf{F} \rangle = \left\langle \oint_S \mathbf{n}\hat{T}\mathrm{d}S \right\rangle, \text{ and } \quad \langle \mathbf{T} \rangle = -\left\langle \oint_S \mathbf{n}(\hat{T}\times\mathbf{r})\mathrm{d}S \right\rangle,$$

where $\hat{T}_{ij} = \left[\varepsilon E_i E_j + \mu_0 H_i H_j - \frac{1}{2}(\varepsilon E^2 + \mu_0 H^2)\delta_{ij}\right]$

Problem of scattering

In order to evaluate the optical force and torque the full electromagnetic field has to be known. We describe the highly focused incident (background) field in analytically using the angular spectrum description [7] in cylindrical coordinates r, θ, z

$$E_x = -\frac{\imath}{2}k\left(I_0 + I_2\cos 2\theta\right), \quad E_y = -\imath k I_2 \sin 2\theta, \quad E_z = -k I_1 \cos\theta,$$

where

$$I_0 = \int_0^{\alpha_a} A_0\sqrt{\cos\alpha}\,\sin\alpha\,(1+\cos\alpha)\,J_0(kr\sin\alpha)\,\exp(\imath kz\cos\alpha)\mathrm{d}\alpha,$$
$$I_1 = \int_0^{\alpha_a} A_0\sqrt{\cos\alpha}\,\sin^2\alpha\,J_1(kr\sin\alpha)\,\exp(\imath kz\cos\alpha)\mathrm{d}\alpha,$$
$$I_2 = \int_0^{\alpha_a} A_0\sqrt{\cos\alpha}\,\sin\alpha\,(1-\cos\alpha)\,J_2(kr\sin\alpha)\,\exp(\imath kz\cos\alpha)\mathrm{d}\alpha,$$

where J_n denotes the Bessel function of the first kind and n-th order. The amplitude A_0 can be related to the electric field intensity at the beam focus $E_x(0,0,0) = \frac{k}{15}A_0\left(8 - 3\cos^{5/2}\theta - 5\cos^{3/2}\theta\right)$.

Comsol Model

- We use *Radio Frequency Module* to solve problem of electromagnetic scattering on gold nanoparticle of triangular decahedral shape
- *Background electric field* is given by the equations above, integration is replaced by the explicit summation (11 terms)
- Numerical aperture of focusing lens is 0.5 (α_a = 21.5 deg)
- Studied geometry consists of metallic object of refractive index n = 0.2851–7.36 $\imath$ (variously oriented) which is enclosed by a spherical medium (refractive index n_m = 1.33) and by a *spherical PML layer*, see figure 3

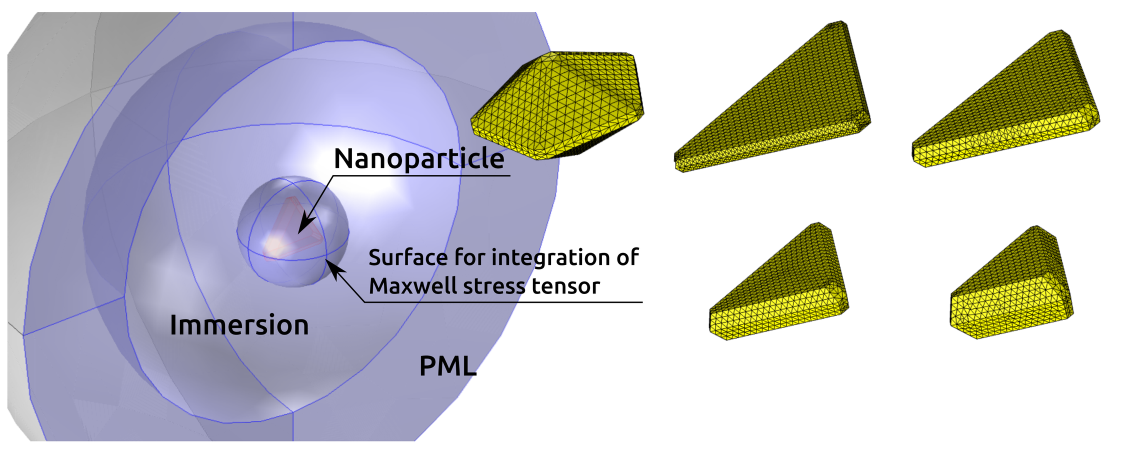

Figure 3: *The model geometry and the shapes of golden nanoparticles – decahedral and triangular plates of various aspect ratios. Note, that all triangular plates have the same volume.*

- up to ~ 75 000 mesh elements, > 500 000 degrees of freedom
- Optical forces and torques are evaluated as Boundary probes. Maxwell stress tensor defined by Comsol Multiphysics is employed
- Power absorbed by the particle is calculated as a volume integral of resistive loses. Temperature increase may be calculated by approximation or using *Heat Transfer Module*
- Various particle locations with respect to incident beam are evaluated using *Auxiliary sweep*. Particle orientations and sizes are studied using *Parametric sweep*

Optical Forces and Torques: Results

We calculated optical forces and torques acting on a decahedron and triangular plate. Both particles have the same volume as the sphere having diameters 100, 150, 200 and 250 nm; we considered the aspect ratios of the object height and circumscribed circle diameter 0.3 for decahedron and 0.15 for triangular plate.
The optical torque orienting particle (tilted by 45 degrees with respect to beam polarization) is plotted in first row of figure 4. Negative T_z orients decahedral particle parallel to polarization (left part of figure 4) while positive T_z orients triangular plate perpendicular to the beam polarization Middle row of figure 4 shows the optical force along beam propagation axis for the particle oriented to its stable orientation. We can see that decahedrons with d_{eff} = 100 and 150 nm are stably trapped and that all sizes of triangular plates are trapped. Bottom row shows electromagnetic power P_{abs} absorbed by the particle in different z.

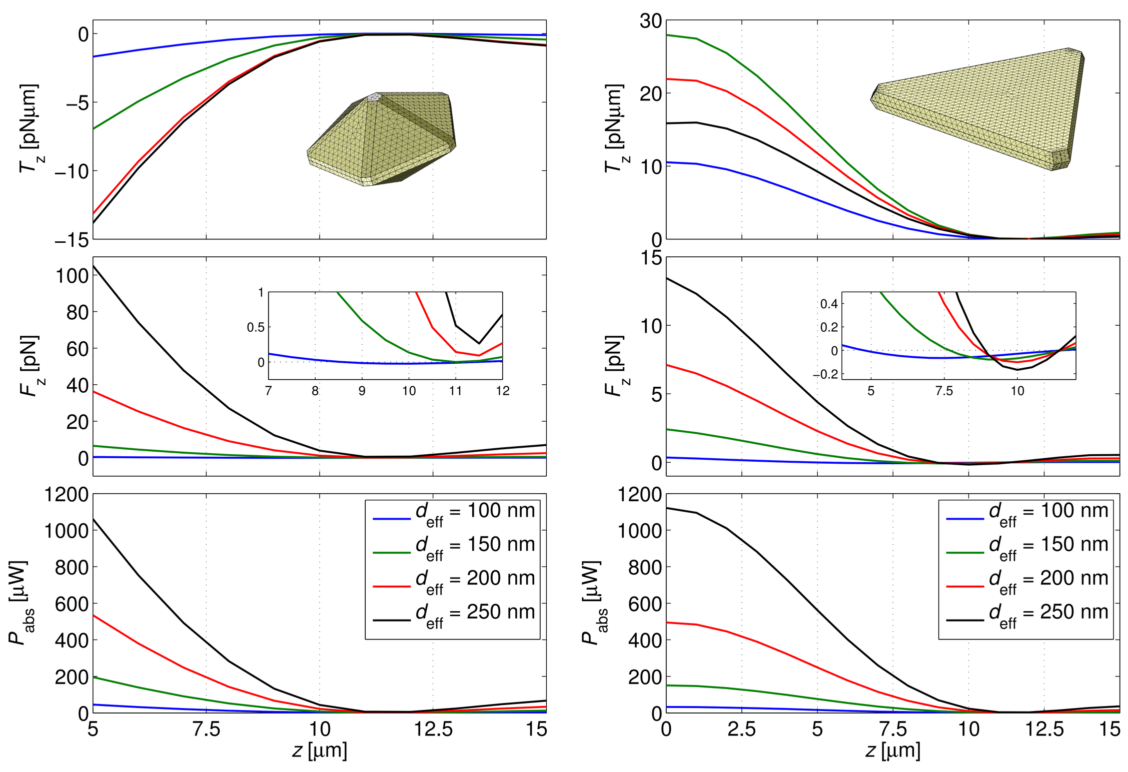

Figure 4: *(top) Optical torques acting on a decahedron (left) or a triangular plate (right) placed in a distance z behind the focal point. The object is 45° tilted with respect to beam polarization. Different colors of curves correspond to d_{eff} = 100 – 250 nm. (middle) Optical force F_z acting on a particle in stable orientation along beam propagation axis. Inset magnifies the negative forces indicating stable trapping. (bottom) Power absorbed by the particles in various positions.*

Further, we calculated the effect of varying the aspect ratio of triangular plate height and the circumscribed circle diameter in order to obtain object stable orientation. Figure 5 shows the optical torque that rotates particle parallel to beam polarization ($T_z < 0$) or perpendicular to beam polarization ($T_z > 0$). Only very flat small object are rotated perpendicular to polarization. Similarly, even thicker and larger objects are still oriented perpendicular to beam polarization. This suggests, that such larger and thicker objects may still be trapped in optical tweezers.

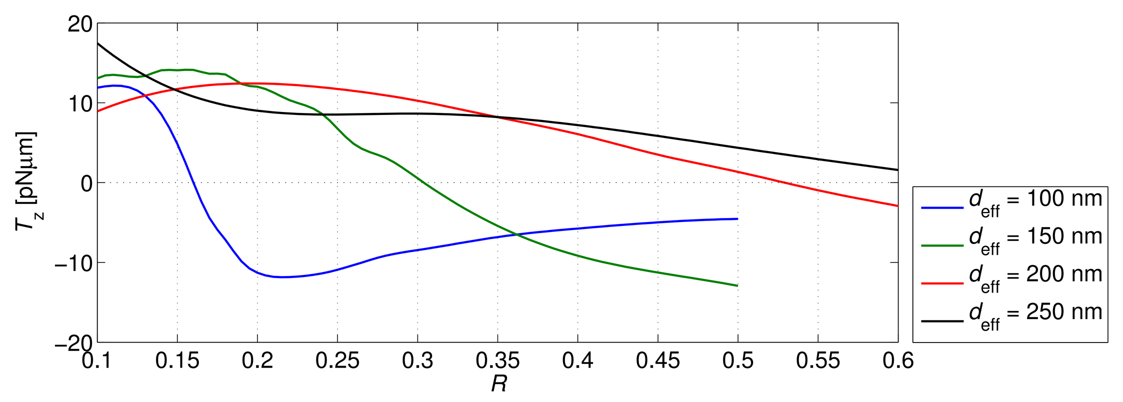

Figure 5: *Optical torques acting on a triangular plate having different aspect ratios of plate height and circumscribed circle diameter. The object is 45° tilted with respect to beam polarization placed in a distance $z = 5\,\mu\mathrm{m}$ behind the focal point. Different colors of curves correspond to effective diameters 100-250 nm of a spheres having the same volume.*

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Acknowledgments

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