Forces and Heating in Plasmonic Particles

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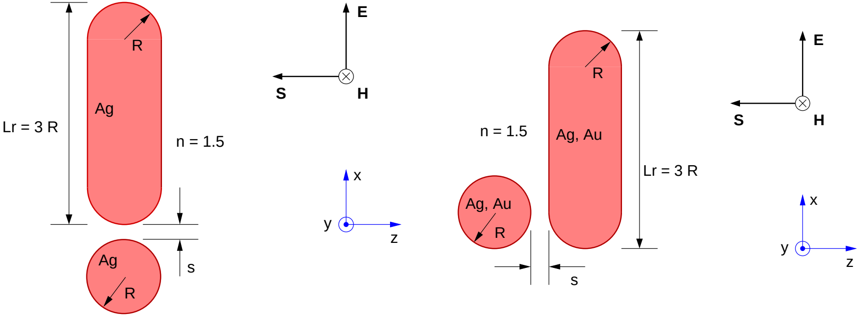
Optical forces at plasmonic particles: geometrical configurations



Excitation plane wave field strength: $|E_0| = 10^6$ V/m

Optical force calculation

The optical force is obtained from the equation of conservation of momentum

$$\frac{d[G_{mech} + G_{em}]}{dt} = \int_{\partial V} \overleftrightarrow{\mathbf{T}} \cdot \mathbf{n} \, dS$$

where

$$T_{ij} = \varepsilon_r \varepsilon_0 E_i E_j + \frac{1}{\mu_r \mu_0} B_i B_j - \frac{1}{2} \left(\varepsilon_r \varepsilon_0 E^2 \delta_{ij} + \frac{1}{\mu_r \mu_0} B^2 \delta_{ij} \right)$$

is the Maxwell stress tensor.

Optical forces near a plasmonic particle

For time-harmonic fields

$$\left\langle \frac{dG_{em}}{dt} \right\rangle_T = 0$$

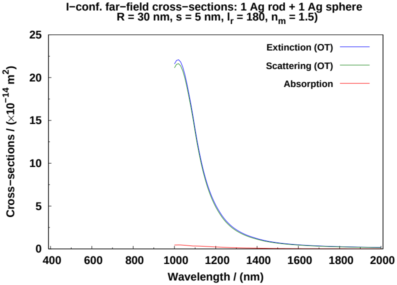
Then, the mechanical force is obtained by

$$\mathbf{F} = \left\langle \frac{dG_{mech}}{dt} \right\rangle_T = \int_{\partial V} \left\langle \overleftrightarrow{\mathbf{T}} \cdot \mathbf{n} \right\rangle dS$$

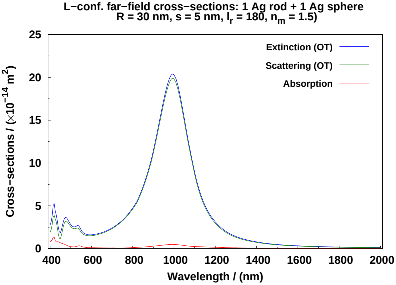
and the trapping potential is

$$U(\mathbf{r}_0 = -\int_{\infty}^{\mathbf{r}_0} \mathbf{F}(\mathbf{r}) d\mathbf{r}$$

Optical forces at plasmonic particles: far-field total cross-sections (Ag)

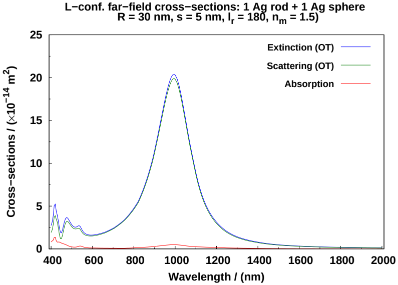


Silver I-configuration

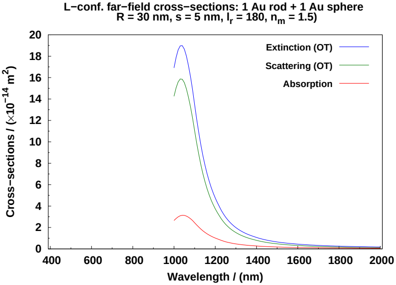


Silver L-configuration

Optical forces at plasmonic particles: far-field total cross-sections (Ag vs. Au)

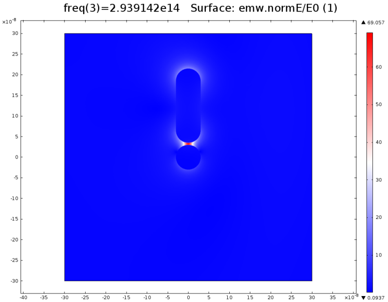


Silver L-configuration

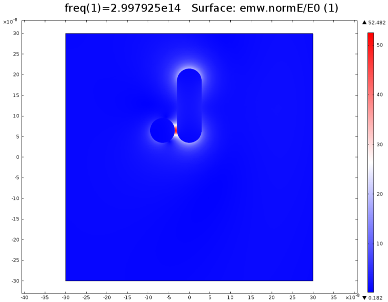


Gold L-configuration

Optical forces at plasmonic particles: near-field (Ag)

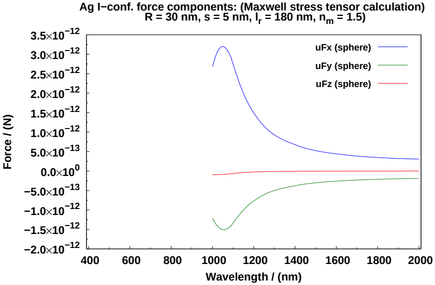


$\lambda = 1020$ nm

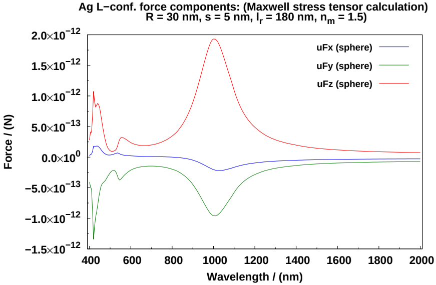


$\lambda = 1000$ nm

Optical forces at plasmonic particles: MST force components (Ag)

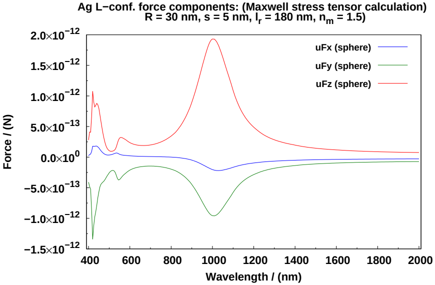


Silver I-configuration

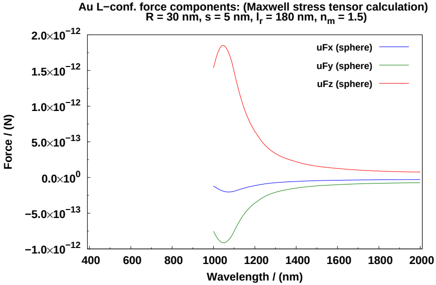


Silver L-configuration

Optical forces at plasmonic particles: MST force components (Ag vs. Au)



Silver L-configuration



Gold L-configuration

Thermal plasmonics

Resistive losses in plasmonic particles generate heat Q

- The temperature distribution close to the particle is governed by

$$\rho c_P \frac{\partial T}{\partial t} + \nabla \cdot (\kappa_S \nabla T) = -q(\mathbf{r}, t)$$

- The transient time τ required to reach the steady state is given by

$$\tau \sim \frac{R^2}{D}$$

  where $D = \kappa/(\rho c_P)$ is the thermal diffusivity. For a sphere of radius $R = 100$ nm in water ($D_{\text{water}} = 1.43 \times 10^{-8}\text{m}^2\text{s}^{-1}$) $\tau \simeq 0.7\mu\text{s}$.

- In the steay-state regime $\nabla \cdot (\kappa_S \nabla T) = -q(\mathbf{r})$. The total heating power is $Q = \sigma_{abs} I_0$, and the maximal temperature for CW illumination is

$$\Delta T_{NP} = \frac{Q}{4\pi R_{eq} \kappa_{\text{water}}}$$

Thermal conductivity of materials

Material	Thermal conductivity: κ / ($Wm^{-1}K^{-1}$)
water	0.58
gold	314
silver	427
silicon (crist.)	149
silicon (amorph.)	1 - 4
quartz (fused silica)	1.38
SL graphene	4800 - 5300 (*)

(*) Balandin et al., "Superior Thermal Conductivity of Single-Layer Graphene", Nano Lett. **8**, 902 (2008).

For a gold sphere ($R = 30$ nm) in water, illuminated by a plane wave with an intensity of 2 mW/µm^2 ($\lambda = 550$ nm, CW) a maximum temperature of $\Delta T \simeq 115$ K can be reached above the temperature of the medium in thermal equilibrium.

Thermal effects on plasmonic particles

The maximum temperature increase is given by

$$\Delta T_{NP} = \frac{\sigma_{abs} I_0}{4\pi R_{eq} \beta \kappa_{water}}, \qquad I_0 = n\epsilon_0 c |E_0|^2/2$$

For the rod, $\beta \sim 1.1$ and $R_{eq} = 47.6$ nm

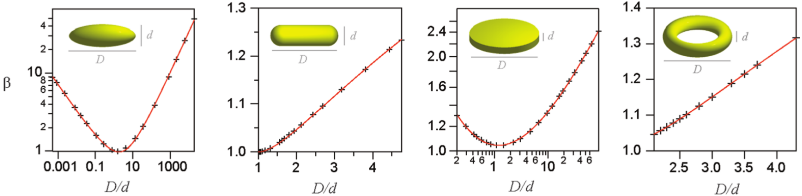


Figure 3. Universal dimensionless thermal-capacitance coefficient β for ellipsoids, rods with hemispherical caps, disks, and rings as a function of their aspect ratio *D*/*d* (see insets). This coefficient relates the temperature increase of an irradiated nanoparticle to the absorption power and the thermal conductivity of the surrounding medium, according to eq 4. We show numerical simulations (symbols) compared to the fitting functions of Table 1 (curves). The value of β is given for a particle of volume equal to that of a sphere of equivalent radius $R_{eq} = (d^2D/8)^{1/3}$ for ellipsoids, $R_{eq} = [(3D - d)d^2/16]^{1/3}$ for rods, $R_{eq} = (3D^2d/16)^{1/3}$ for disks, and $R_{eq} = (3\pi d^2D/16)^{1/3}$ for rings.

Baffou, Quidant, García de Abajo, “Nanoscale control of optical heating in complex plasmonic systems”,

ACS Nano **4**, 709 (2010).

Remarks

- Ag and Ag NPs can trap other NPs, reaching optical forces of several pN at intensities of ~ 2 mW/μm^2
- Au NPs can generate large temperature gradients, when excited at the plasmon resonances
- Temperature simulations will be done to confirm the predicted temperature increase
- COMSOL Multiphysics MST forces calculation work fine on v4.2a
- COMSOL Multiphysics MST forces calculation fail on v4.3a and v4.3b

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