Heating of metal nanoparticles on absorbing substrates

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INTRODUCION

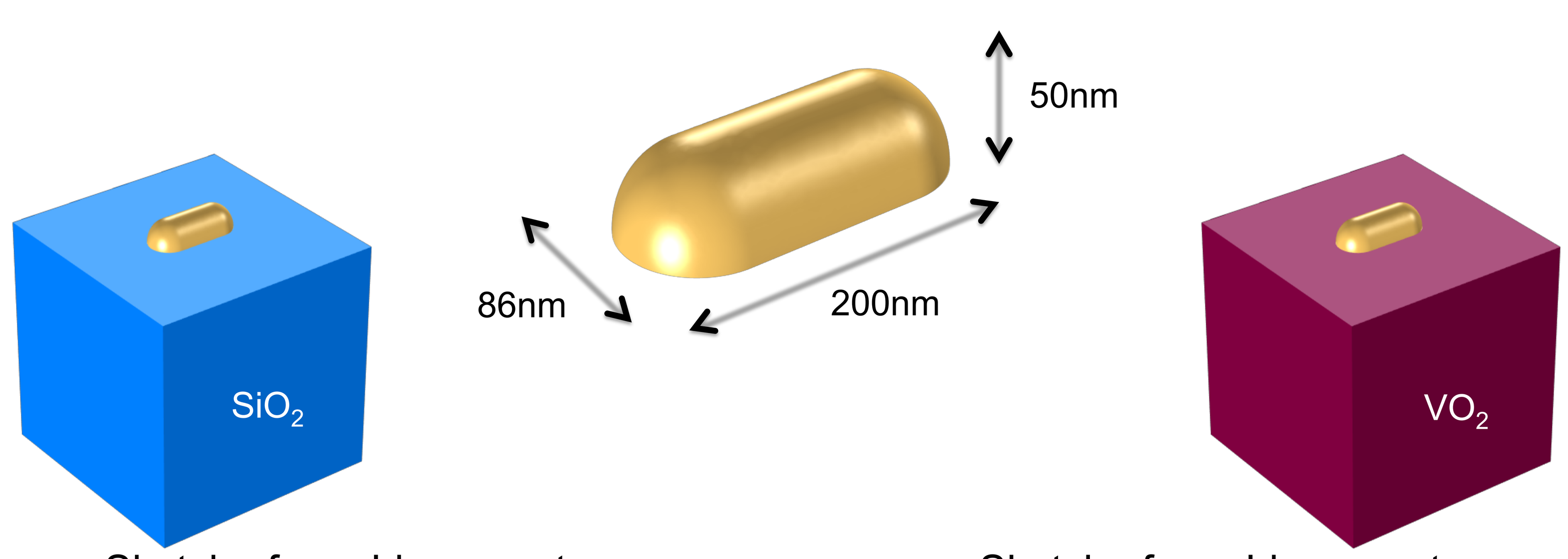
Metal nanoparticles (NPs) are known to host collective excitations of the conductive electrons (plasmons) under illumination in the Visible-NIR spectrum [1]. Between the effects of such excitations there is a heating up of the NPs themselves due to a Joule effect process [2]. The produced heat diffuses in the surrounding producing an increase in the temperature of the neighboring media. The usual setup of an experiment involves the realization of NPs on a substrate, which is often optically non-absorbing (e.g., glass) [3]. In this case analytical and numerical methods are already available to handle such a system based on the assumption that the only heat sources in the system are the NPs [2].

What happens if also the (light-absorbing) substrate produces heat? Furthermore, how does the temperature profile change in the surrounding of the NPs?

To answer these questions we exploited the multiphysics capacity of COMSOL software.

CASE AT HAND

We studied the case of a Gold nanoantenna (AuNA) on both SiO_2 (optically non-absorbing) and VO_2 (optically absorbing) substrate. The NA is illuminated with $0.5 \cdot 10^8 W/cm^2$ intense laser for 10ps and then the temperature profile around the NA is observed 40ps after the light switching off.



Sketch of a gold nanoantenna on the top of a non-absorbing substrate (SiO_2)

Sketch of a gold nanoantenna on the top of an absorbing substrate (VO_2)

COMPUTATIONAL METHODS

The study is performed with a 2-steps simulation:

1st step) Optical simulation for an impinging plane-wave at a wavelength of λ=1060nm

We use the "Electromagnetic Waves, Frequency Domain" interface to solve the Maxwell equations with "PML" boundary conditions

$$\nabla \mathbf{D} = 0 \qquad \nabla \times \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}$$

$$\nabla \mathbf{B} = 0 \qquad \nabla \times \mathbf{H} = \frac{\partial \mathbf{D}}{\partial t}$$

$\mathbf{E}$ = electric field vector
$\mathbf{B}$ = magnetic induction vector
$\mathbf{D}$ = displacement field vector
$\mathbf{H}$ = magnetic field vector

2nd step) Thermal simulation when undergoing a pulse illumination

We solve the heat diffusion equation in the time-space with open boundary conditions via the "Heat Transfer in Solids" module

$$\rho C_P \frac{\partial T}{\partial t} - \nabla \cdot \left(k \nabla T\right) = Q$$

ρ = material density
C_P = material heat capacity at constant pressure
k = material thermal conductivity
Q = heat density source

The heat density source is set as

$$Q = \frac{\omega}{2} \mathrm{Im}\left\{\mathbf{P}^* \cdot \mathbf{E}\right\} \qquad t \le 10\,ps$$

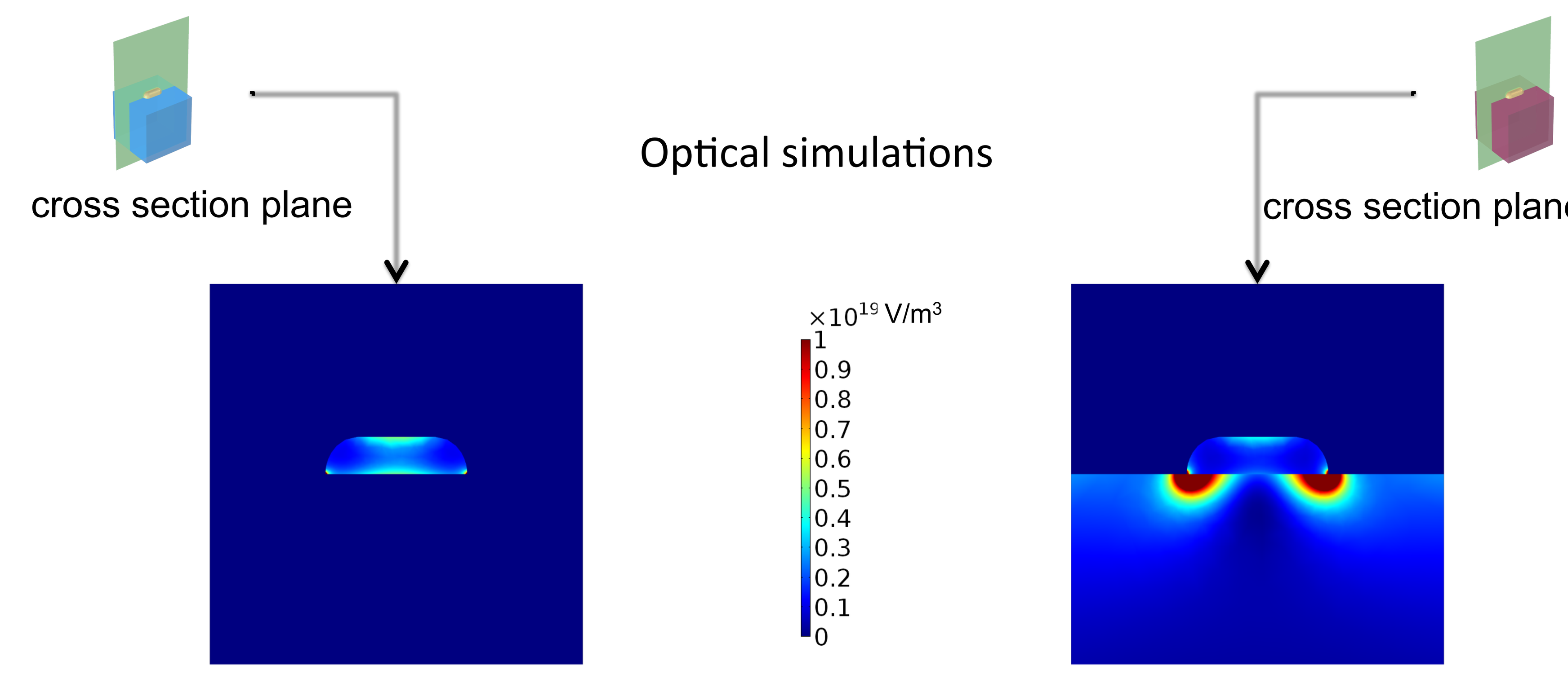
$$Q = 0 \qquad t > 10\,ps$$

ω = frequency corresponding to illuminating λ

where the polarization vector (**P**) and the electric field vector (**E**) are taken from the optical simulation (i.e., first step).

RESULTS

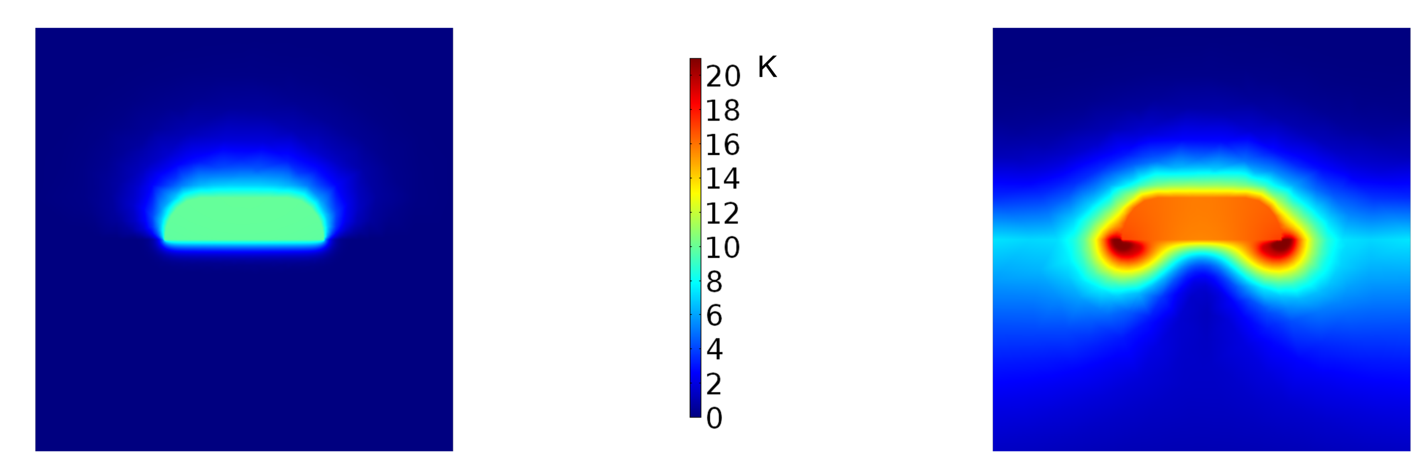
Optical simulations



Heat density source (Q) distribution for a non-absorbing substrate

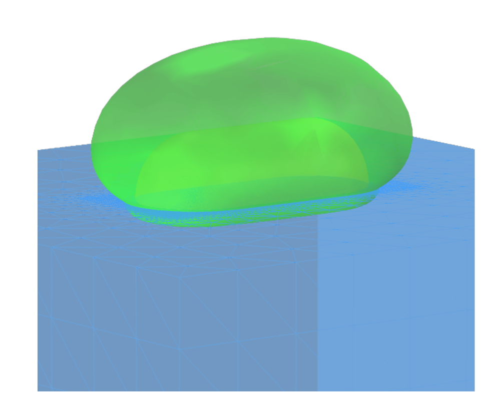
Heat density source (Q) heat distribution for an absorbing substrate

Thermal simulations

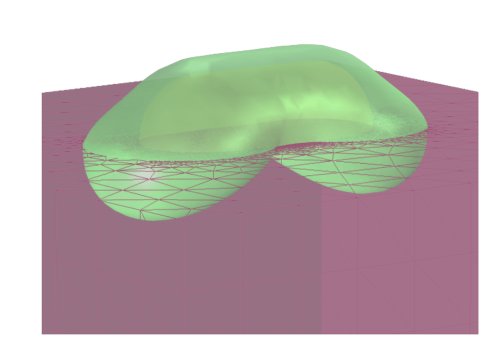


Distribution of the temperature increase (ΔT) around the NA for a non-absorbing substrate

Distribution of the temperature increase (ΔT) around the NA for an absorbing substrate



3D-temperature distribution around the NA for a non-absorbing substrate isosurface of ΔT = 2K



3D-temperature distribution around the NA for an absorbing substrate isosurface of ΔT = 10K

CONCLUSIONS

- ✓ We successfully combined the optical and thermal modules of COMSOL MULTIPHYSICS
- ✓ We exploited both a stationary and time-dependent solution
- ✓ The temperature distribution in the absorbing substrate is remarkably different with respect to the non-absorbing one
- ✓ The temperature increase of both the NP and the surrounding is enhanced

REFERENCES

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