Effective modeling for hybrid nanoscale platforms: multi-modal photothermal and MRI applications

C. Rousseau[1] , Q.L. Vuong[2] , Y. Gossuin[2] , B. Maes[1] and G. Rosolen[1]

[1]Micro- and Nanophotonic Materials Group, Research Institute for Materials Science and Engineering. University of Mons, 20 Place du Parc, B-7000 Mons, Belgium

[2]Biomedical Physics Unit. University of Mons, 20 Place du Parc, B-7000 Mons, Belgium

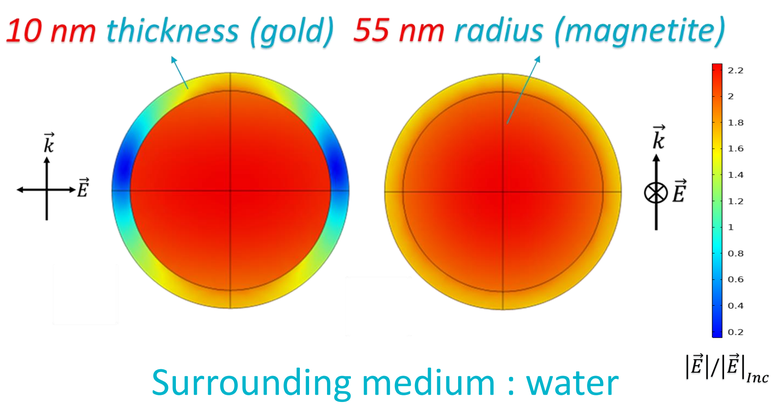
UMONS University of Mons

Abstract

Recently, hybrid nanoplatforms combining iron oxide and gold materials have been developed for their simultaneous use in magnetic resonance imaging and plasmonic photothermal therapy. Submitted to a continuous-wave (CW) laser illumination, these hybrid nanoparticles absorb and convert some of the incident energy into heat. In this study, we investigate both the temperature gradients involved when a single nanoparticle is placed under CW laser illumination, as well as when a group of nanoparticles is subjected to the same illumination. These temperature gradients can have an impact on the transverse relaxation time in magnetic resonance imaging (MRI).

Structure

- Hybrid nanoplatforms → Nanoshell



Surrounding medium : water

Plasmonic resonance → λ = 865 nm

Theoretical model

- Analytical expression of the temperature profile (in the surrounding medium of the NP) :

$$T_{ext}(r) = \frac{Q_{core} + Q_{shell}}{4\pi r \kappa_s} + T_\infty \quad \text{with} \quad Q = \frac{\omega}{2}\varepsilon_0\, Im(\varepsilon_\omega) \iiint_{V_{NP}} |E_\omega|^2\, dV$$

Distance to NP surface — Surrounding thermal conductivity

Single NP → $T_\infty = T_{amb}$ Multiple NPs → $T_\infty = T_{collective}$

- The collective thermal model [1] :

$$T_{collective}(\vec{r}) = \iiint_{Beam_{laser}} \frac{q(\vec{r'})}{4\pi\kappa_s |\vec{r'} - \vec{r}|} dr' \quad \text{with} \quad q(\vec{r'}) = I_0\, N\, \sigma_{abs}\, e^{(-\sigma_{ext} N z)}$$

Heat power density — NP absorption cross section — Distance in sample — NP extinction cross section

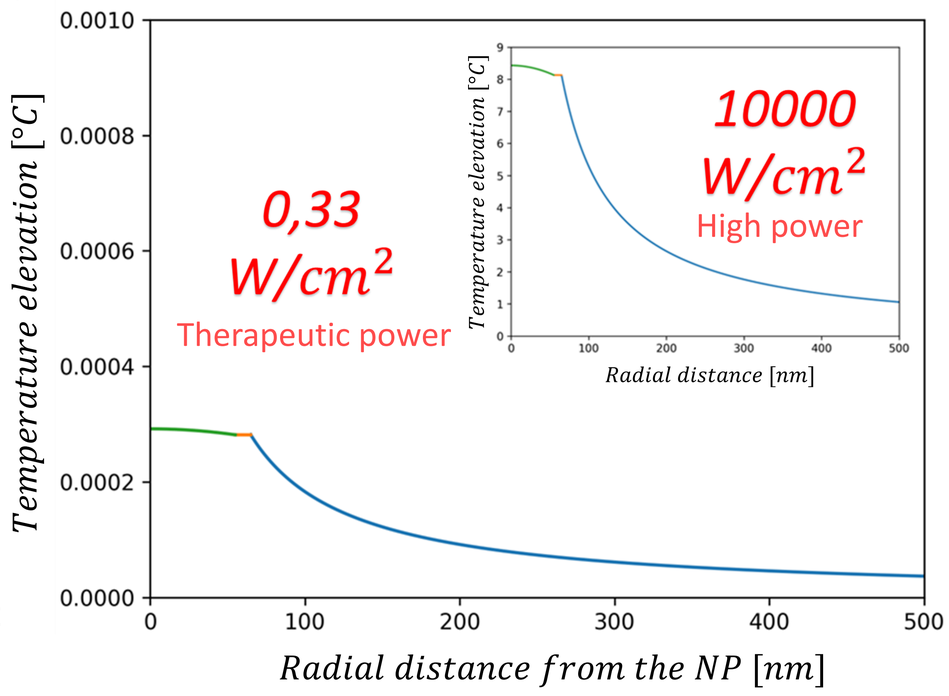
$|E|$, σ_{abs} and σ_{ext} obtained via COMSOL simulations

Temperature profile for a single nanoshell

- Nanometer scale gradient with small temperature changes at therapeutic laser power.

It does not explain the temperature rise in experimental results [2]!
+
The effect on proton relaxation in MRI is negligible.

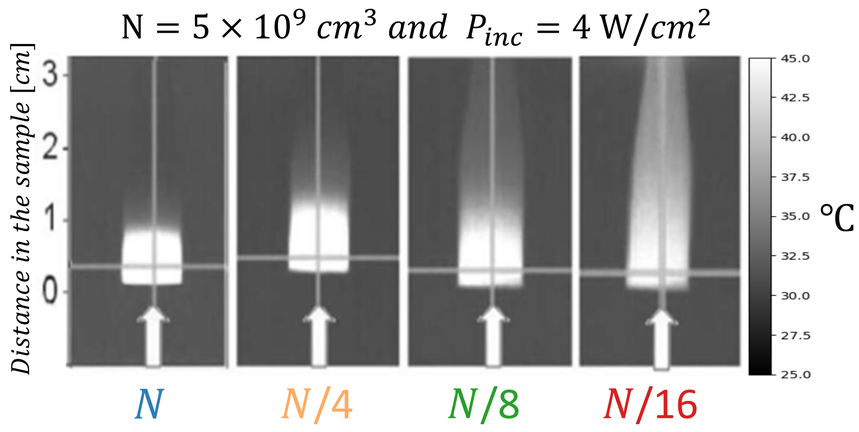
- Non-negligible gradient appears with high laser power.



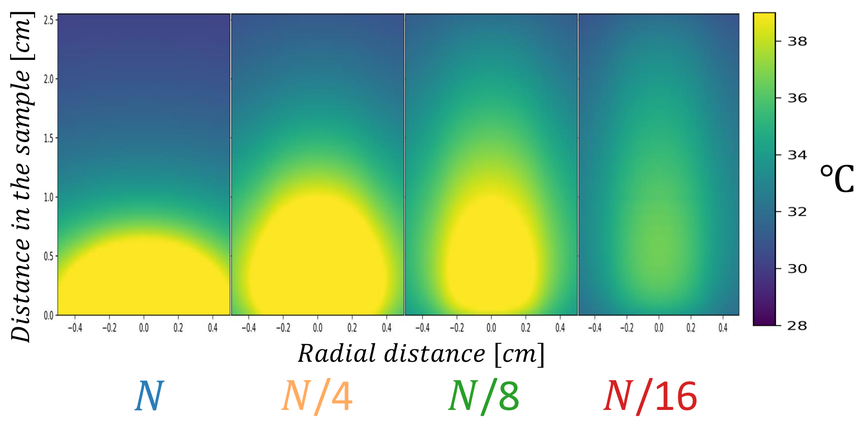
Collective model

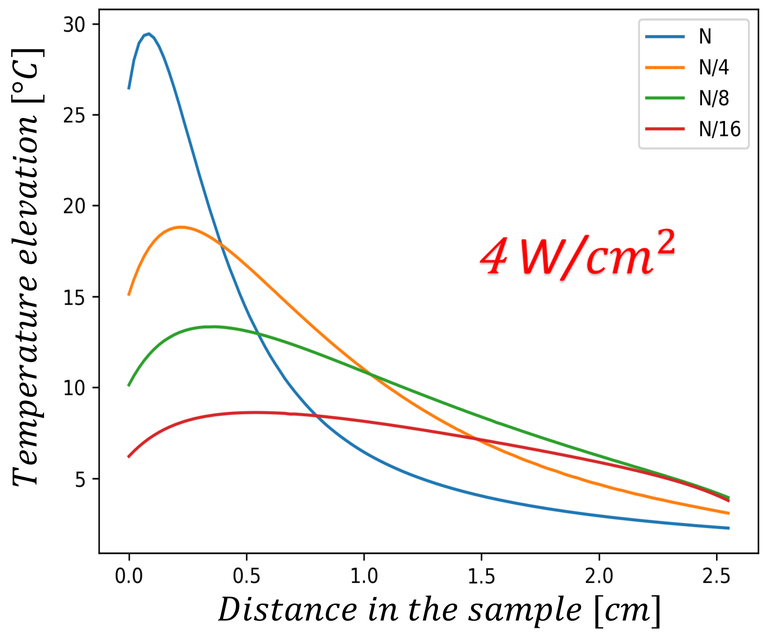
- Experiment : solution of silica/gold nanoshells (140/20 nm) in physiological solution heated with a 810 nm laser (blank arrow). [2]

$N = 5 \times 10^9\ cm^3$ and $P_{inc} = 4\ W/cm^2$



- Theoretical collective thermal model :

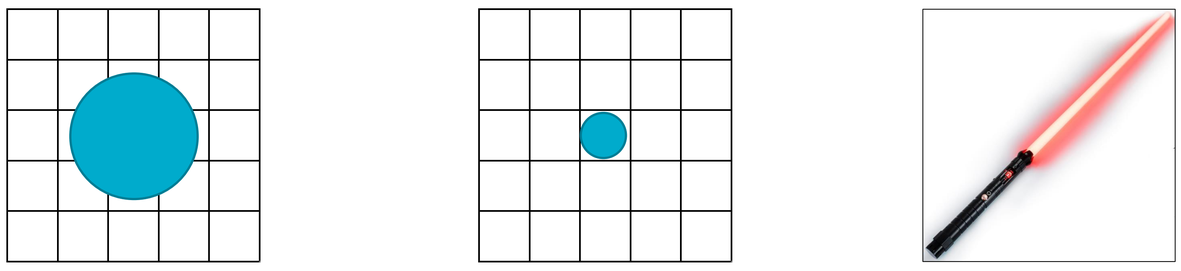




cm scale gradient with strong temperature changes → impact in MRI

Conclusion and outlook

- The temperature gradient at the single NP size is too weak to have an impact on the transverse relaxation time in magnetic resonance imaging, except with a very high laser power.
- The temperature gradient generated inside a solution of particles, by the beam itself can, however, have a significant impact.
- The impact of temperature gradients on the MRI contrast, due to changes in transverse relaxation time will be measured for three configurations :



$Beam_{laser}$ > Size MRI pixel — $Beam_{laser}$ < Size MRI pixel — $Power_{laser} > Power_{medical}$

[1] G. Baffou, Thermoplasmonics: Heating Metal Nanoparticles Using Light, Cambridge: Cambridge University Press, 2017.
[2] Terentyuk et al. « Laser-Induced Tissue Hyperthermia Mediated by Gold Nanoparticles: Toward Cancer Phototherapy ». Journal of Biomedical Optics 14, n° 2 (2009).

Contact: cedric.rousseau@umons.ac.be

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