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Numerical Investigation of Gold Nanoshell Heating Dynamics for Optimized Nanoshell-Assisted Cancer Photothermal Therapy

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INTRODUCTION & AIM

Gold nanoshells (AuNSs) have emerged as powerful agents in biomedical imaging and cancer photothermal therapy (PTT) due to their remarkable ability to convert optical energy into heat through localized surface plasmon resonance. Their tunable optical properties enable precise targeting of tumors while minimizing damage to surrounding tissues [1 - 3].

The aim of this work is to analyze and compare the photothermal heating behavior of SiO_2@Au and $BaTiO_3$@Au nanoshells by employing the Finite Element Method (FEM) using COMSOL Multiphysics. Through coupled electromagnetic and thermal simulations, the study investigates how nanoshell composition, shell geometry, and laser pulse duration influence temperature rise. This approach provides a quantitative basis for optimizing $BaTiO_3$@Au nanoshells as highly efficient and controllable agents for photothermal cancer therapy.

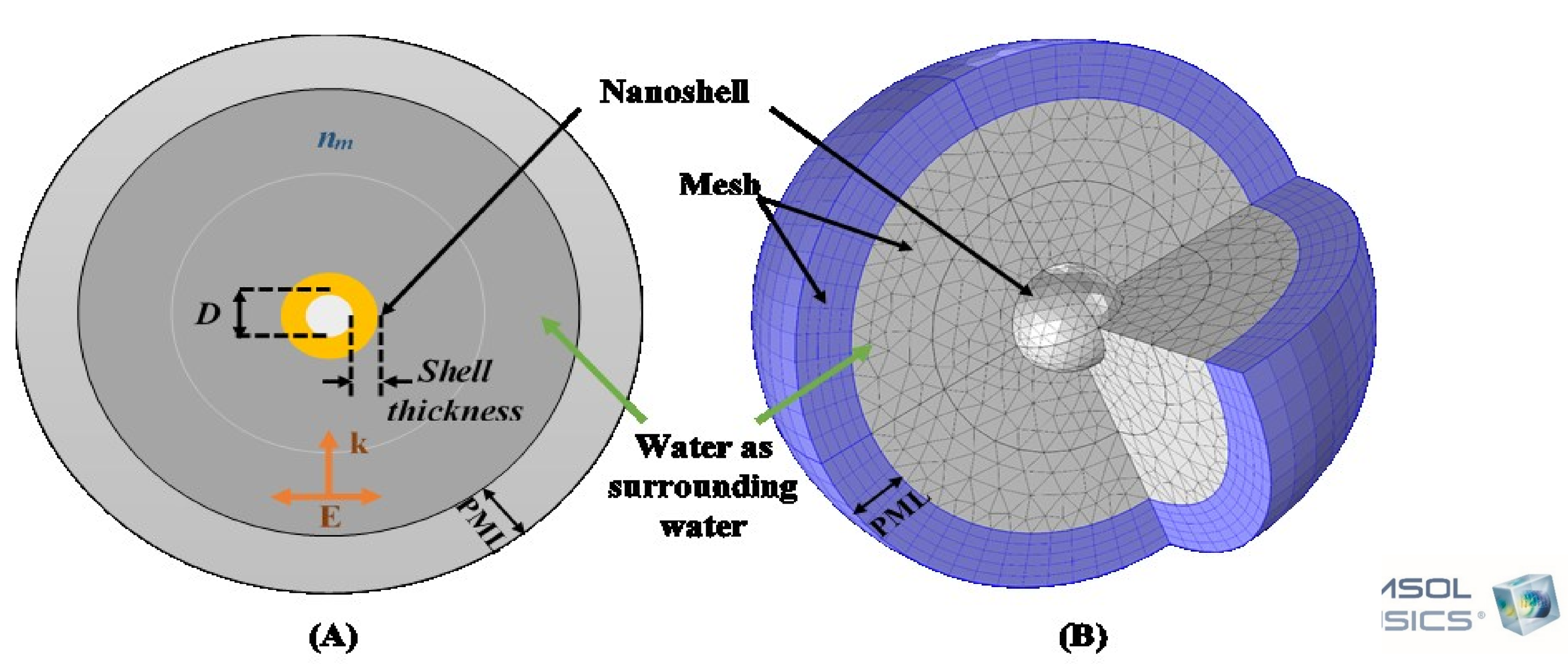
METHOD

Using the Finite Element Method (FEM) in COMSOL Multiphysics, we modeled the electromagnetic absorption and resulting heat generation of SiO_2@Au and $BaTiO_3$@Au nanoshells. Core–shell geometry, optical properties, and heat transfer in the surrounding medium were fully incorporated. Temperature evolution was simulated under two laser excitation regimes: CW and nanosecond pulses, allowing assessment of how pulse duration, shell thickness, and fluence affect each nanoshell's photothermal performance.

$$\sigma_{abs} = \left(\frac{1}{2}\iiint \mathcal{R}e\,(J\cdot E^* + j\omega B\cdot H^*)\right)\Big/ I_0$$ **Absorption cross section**

$$Q_s = (C_{abs} I_0)/V_p$$ **Heat source. Where:** $$I_0(t) = \frac{F_L}{\sqrt{2\pi}t_\sigma}\exp\left(\frac{-[t-t_0]^2}{2t_\sigma^2}\right)$$

$$C_s\rho\frac{\partial T}{\partial t} + \nabla\cdot(-k\nabla T) = Q_s$$ **Heat transfer equation**



RESULTS & DISCUSSION

Figure 1: Cross section ration (Sca / Abs) calculated at a wavelength of 800 nm for SiO_2 and $BaTiO_3$ cores and different gold thickness.

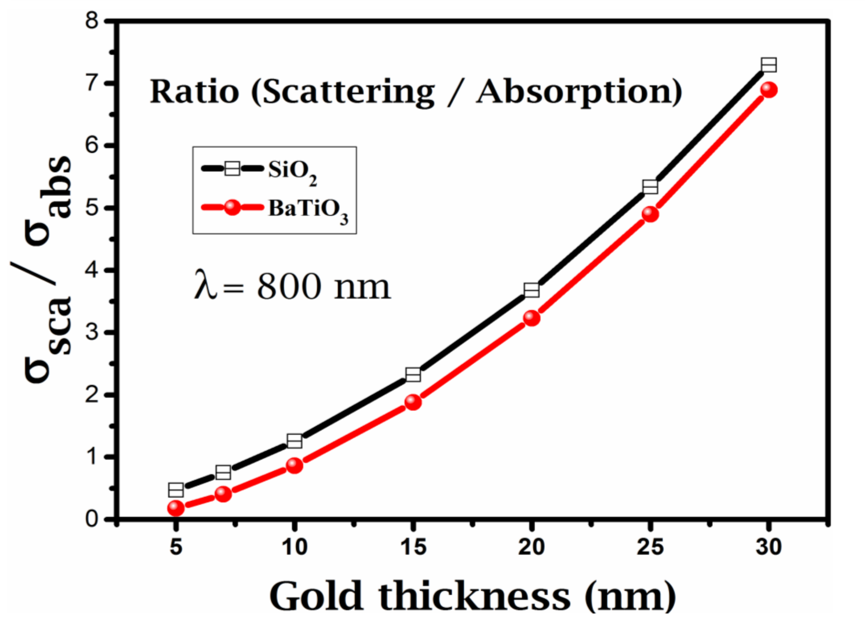


Figure 2: Shift of the LSPR wavelength as a function of the gold shell thickness with a core diameter of 50 nm for SiO_2 and $BaTiO_3$.

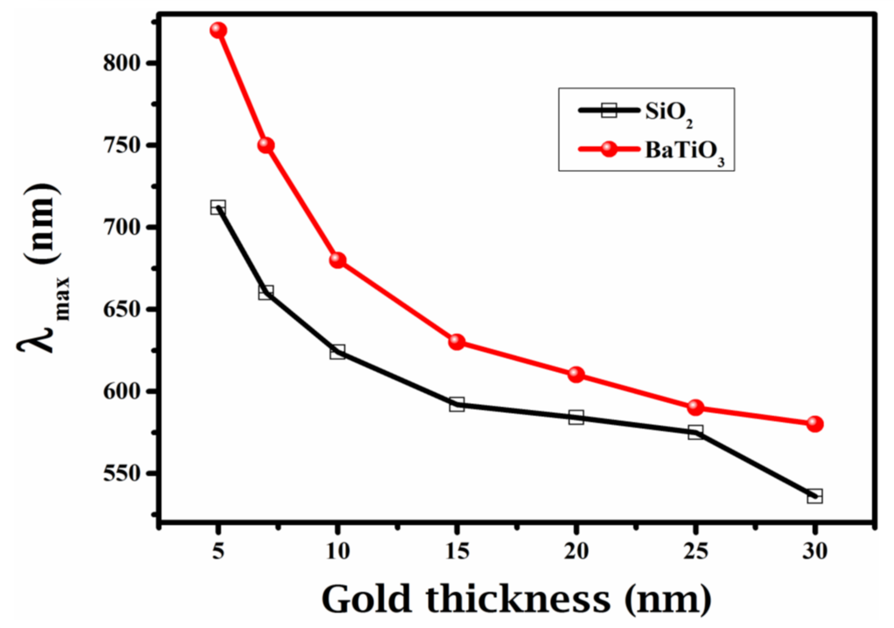


Figure 3: Time profile of the temperature rise on the surface of (A) BaTiO3@Au and (B) SiO2@Au irradiated by CW laser. (C) and (D) Temperature distribution for gold nanoshells with a thickness of 5 nm.

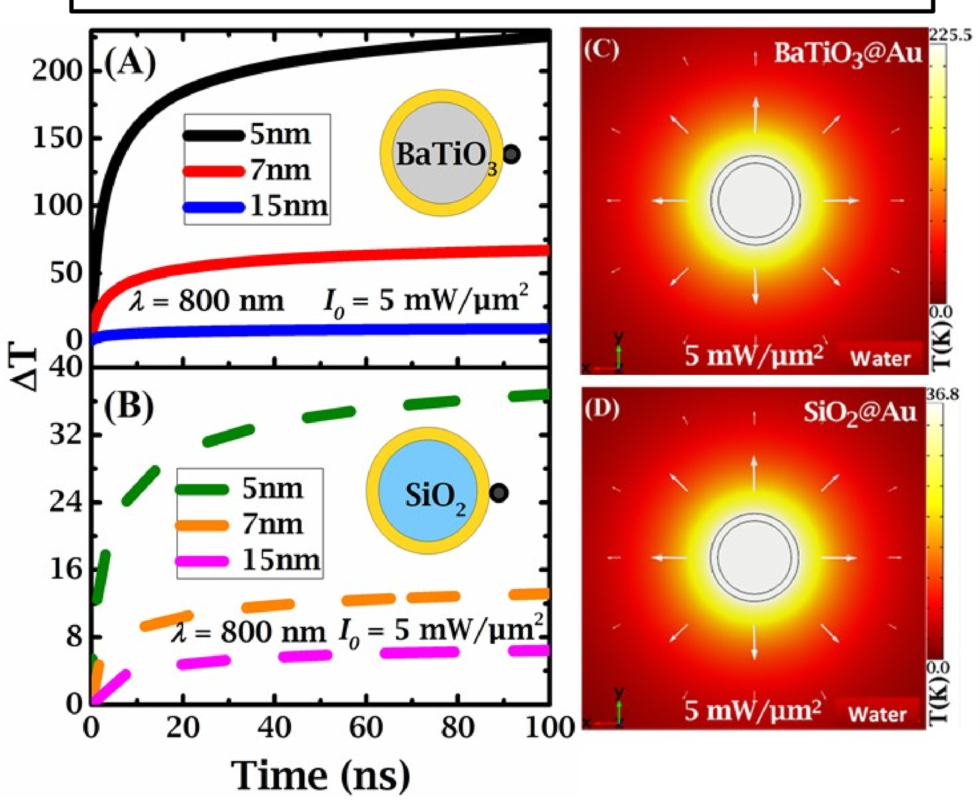


Figure 4: Maximum temperature increase at the surface of gold nanoshells inserted in water as a function of the intensity of the incident CW Laser.

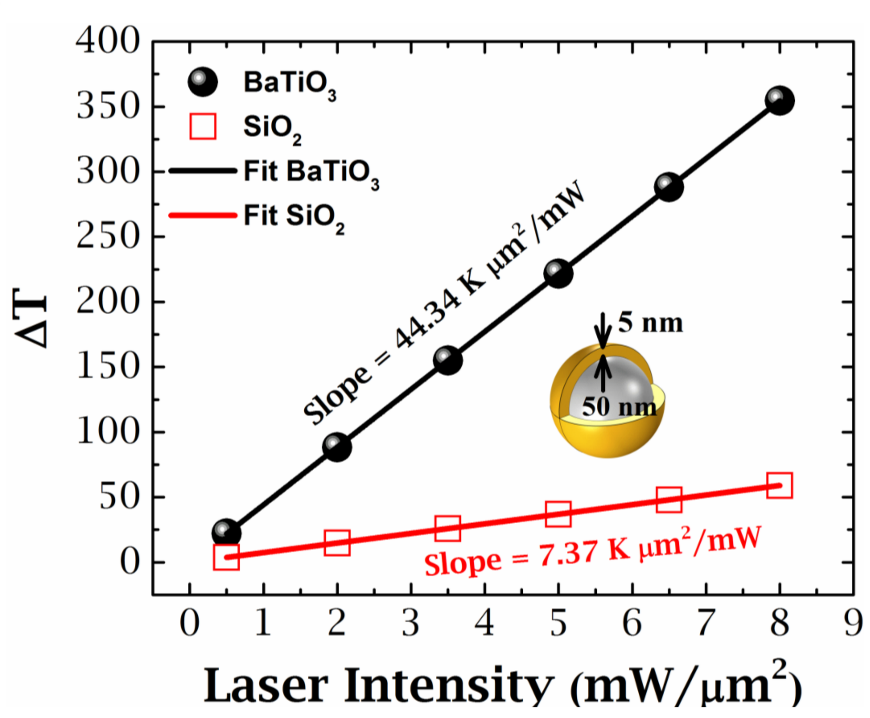


Figure 5: Time profile of the temperature rise on the surface of (A) BaTiO3@Au and (B) SiO_2@Au irradiated by a nanosecond laser pulse. (C) and (D) Temperature distribution for gold nanoshells with a thickness of 5 nm.

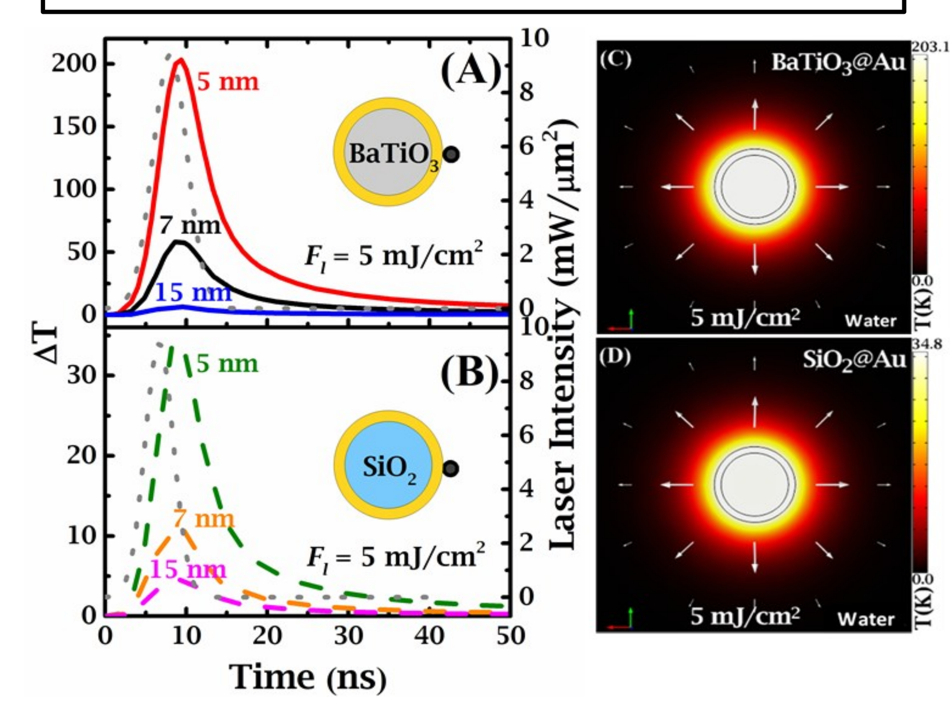
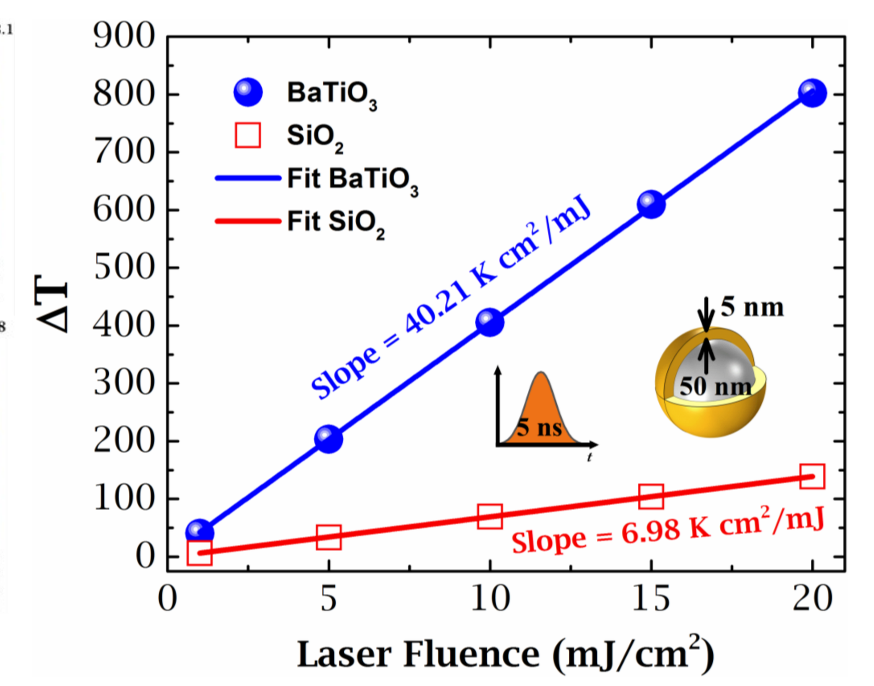


Figure 6: Maximum temperature increase at the surface of gold nanoshells inserted into water irradiated by a nanosecond laser pulse as a function of laser fluence.



CONCLUSION

- $BaTiO_3$@Au nanoshells show significantly higher photothermal performance compared to SiO_2@Au due to their enhanced optical absorption.
- Under ns-laser excitation, $BaTiO_3$@Au reaches much higher temperature rises than SiO_2@Au. Specifically, for a fluence of 5 mJ/cm² and a 5 ns pulse.
- Reducing the laser pulse width into the nanosecond or femtosecond regime leads to highly localized and sharply peaked temperature increases, which are beneficial for precise photothermal therapy with minimal collateral damage.

FUTURE WORK / REFERENCES

Future studies will explore alternative core–shell architectures and optimized geometries to further enhance photothermal efficiency. In addition, extending the modeling to tissue-level heating will help predict clinical treatment conditions more accurately

[1] Badir, A., Refki, S., Sekkat, Z. **Heliyon.**, 11, e42738 (2025)
[2] Gao, X., Li, X., Phan, S., et **al.J. Col & Inter. Sci.**, 645, 907-918 (2023)
[3] Daoudi, C., Ould-Metidji, M., et al. **Eur. Phys. J. Phys.** 82, 20401 (2018)