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Thermal kinetics of Gold Nanosphere under a Burst of Femtosecond laser

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Presentation plan

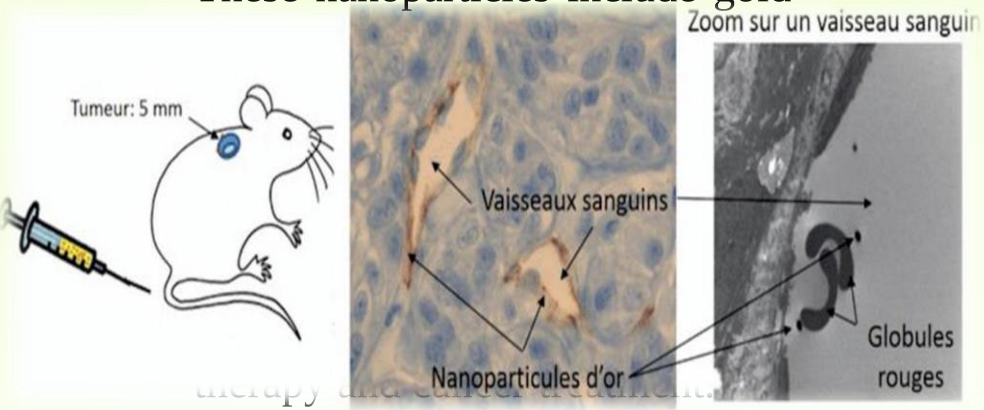
- Introduction
- Modeling of ultra-short pulses
- Gold nanoparticles
- Two temperature model
- Results
- Conclusion and perspectives

Introduction

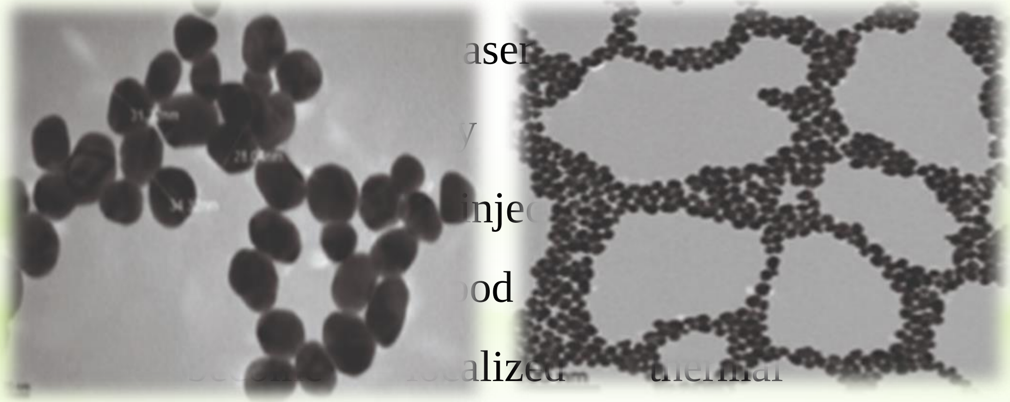
The subject deals with the study of the thermal dynamics that occur within metal nanoparticles following interaction with a laser-like light wave with ultra short pulsed laser . The interaction between a pulsed laser and nanoparticles is of great interest for several sectors including biology and nanomedicine. The fields of application of nanoparticles and ultra-short pulse lasers are booming.

Interest

- These nanoparticles include gold



- The photonic energy emitted by a



destruction agents for cancer cells.

Our work

In this work, we are interested in giving a descriptive analysis of the dynamics of ultra-fast thermal exchanges in a gold nanoparticle, using the two temperature model (TTM).

In order to model the pulse laser/gold nanoparticles interaction, we will consider the following:

*A single femtosecond duration pulse and multipulse.

*A single spherical nanoparticle of diameter D,

The gold nanoparticle is assumed to be placed in water.

Modeling a single ultra-short pulse and pulse train

- Pulse lasers emit very brief photonic radiation called pulses.
- ***The pulse duration τ_p calculated at half-max and the pulse period T can be adjusted.***
- ***burst is a train of pulses with a very short separation time t_{sep} between the sub-pulses.***
- There is a series of mathematical functions that can model a single pulse and the pulse train, the Gaussian type mathematical function is the most appropriate.

$$f(t) = \sum_{i}^{N} 2\sqrt{\frac{ln2}{\pi}}\, e^{-4\, ln(2)\, t^2/\tau_P{}^2}$$

τp: The pulse duration

N: number of pulses per burst

t: Time

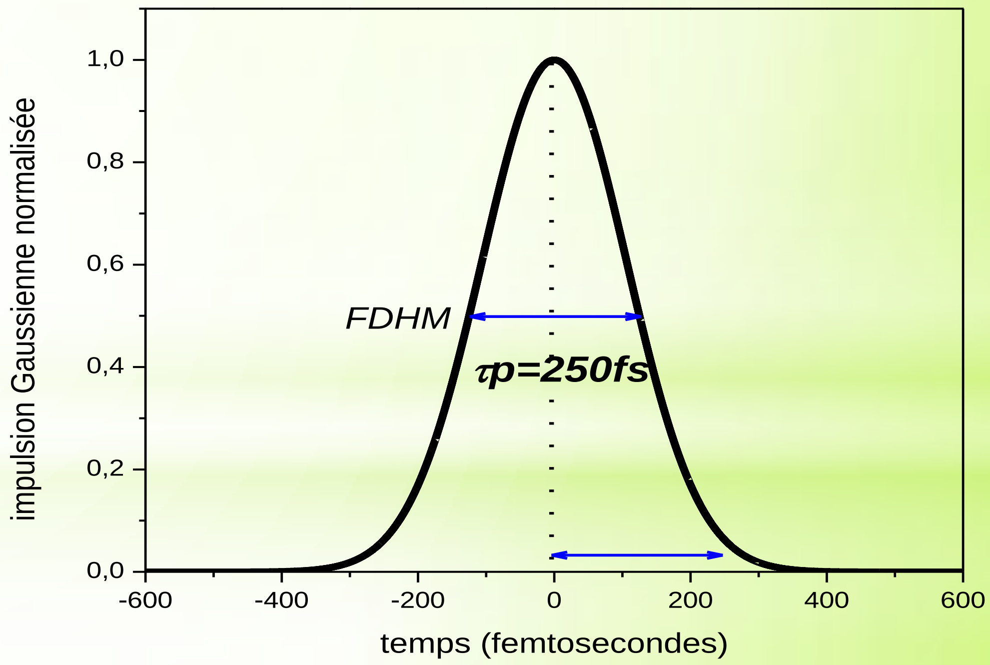


Figure 1: Gaussian time profile of a single femtosecond pulse.

Gold nanoparticles

- A gold nanoparticle (GN) is a group of tens to millions of atoms; its size is between 1 and 100 nm.
- the massive state and the nanoscale state have completely different characteristics. The metallic nanoparticles notably from Au possess in addition to new chemical properties (excellent catalyst etc.):
  - outstanding optical properties,
  - localized thermal properties.

➢ ***The two optical and thermal properties are strongly linked.***

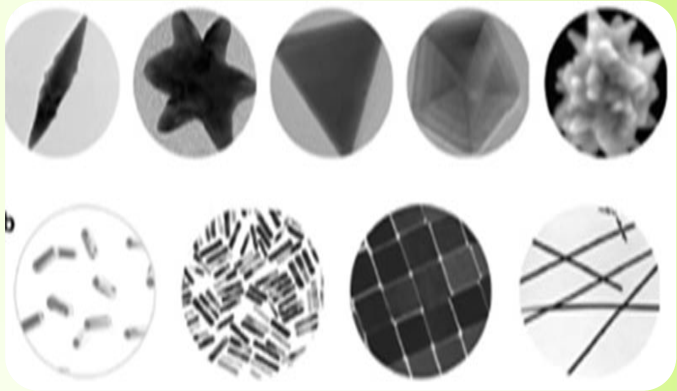


Figure 2 : Différentes formes de nanoparticules synthétisées.

Figure 3 : Coloration des solutions d'or de différentes tailles.

Optical properties of gold NP

When a gold nanoparticle interacts with a light wave (laser) of wavelength λ (or frequency ω), it occurs:

1. A strong extinction of light composed of::

- High absorption of photonic energy in the visible spectrum.
- A diffusion of light that decreases as the size of the nanoparticle decreases.

2. A surface resonance plasmon (SPR) describing the dipolar character of the nanoparticle (collective oscillations of the electronic cloud of quasi-free electrons).

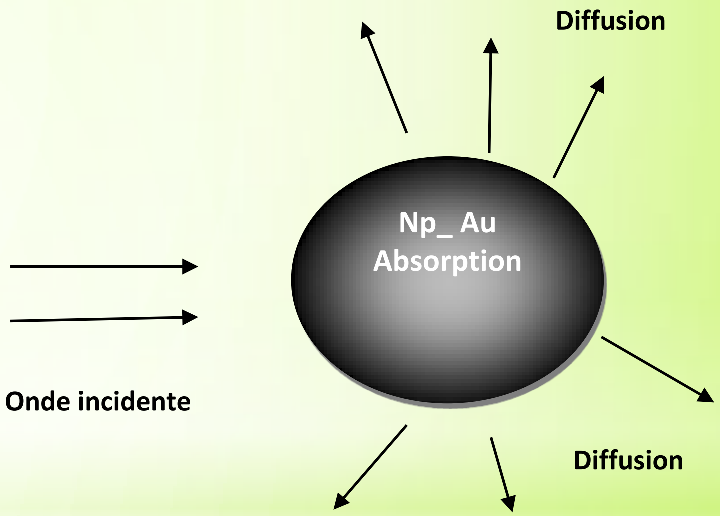


Figure 4: Metallic nanoparticle subjected to a light wave.

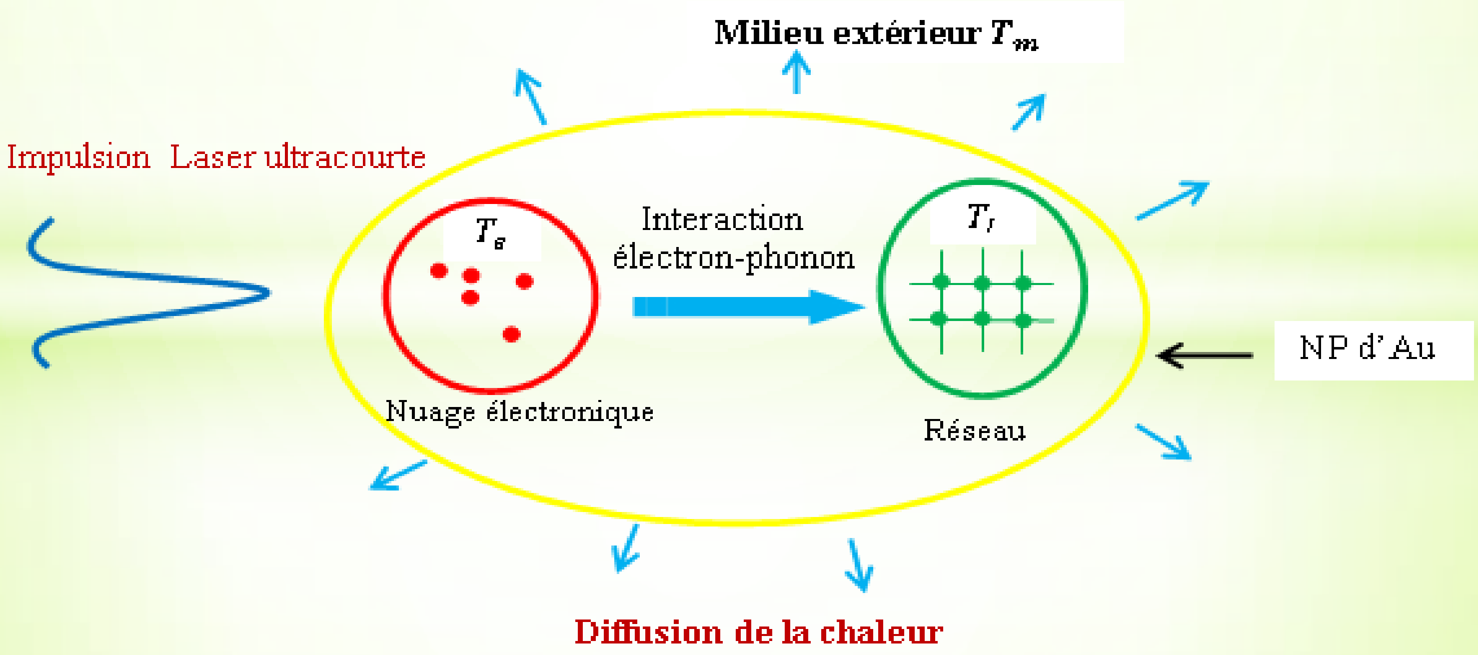
Thermal properties of gold NP

When a gold NP undergoes laser pulses, a very fast thermal dynamic occurs inside the NP.

Phase1:the absorbed photonic energy first excites the free electrons, thus causing a state of out of equilibrium ⇨ **an increase in electronic temperature.**

Phase 2: electrons regain equilibrium by transferring their energy to the crystalline network. ⇨ **an increase in network temperature (lattice).**

the final phase : the nanoparticle releases energy outwards. ⇨ **Cooling of the nanoparticle and heating of the surrounding environment.**



Two temperature model

The two temperature model (TTM) allows to model the exchanges between the two subsystems in the metallic nanoparticle:

- The first electronics;

- the second phononic

The process of thermal exchanges in the nanoparticle is described by a TTM consisting of two coupled differential equations:

$$\begin{cases} C_e(T_e)\,\frac{\partial T_e(t)}{\partial t} = -g(T_e - T_L) + S(t) \\ C_L(T_L)\,\frac{\partial T_L(t)}{\partial t} = g(T_e - T_L) - Q_C \end{cases} \quad (1)$$

$$S(t) = \frac{1}{V_P}\frac{A_{abs} \times F_P}{\tau_P} \times f(t)\,, \quad (2)$$

$$Q_C = 2\pi R k_\infty T_\infty \left(\left(\frac{T_L(t)}{T_\infty}\right)^2 - 1\right), \quad (3)$$

$$Q_C = G\, S_p(\,T_L(t) - T_{ws}(t)),$$

$T_e(t)$ and $T_L(t)$ are the electron and lattice temperatures, respectively;

$C_e(\,T_e)$ and $C_L(\,T_L)$ their specific heats respectively, they depend on the temperatures;

g is the electron-phonon coupling factor, and

S(t) is the energy source generated by the laser in Np.

Q is the term of thermal energy loss.

Numerical resolution method

The resolution of the TTM system is based on the 4-order Runge Kutta numerical scheme which allows to solve ordinary differential equations.

- Initial values are required to start the algorithm (at $t=0$, $T_e=T_L= T_{ws} =300$ K).
- We simulated thermal dynamics by considering a single Gaussian profile multipulse.

Simulation data

laser parameters			
pulse duration	τ_p	$(\mathbf{ps})$	$\tau_p = 100$
Laser fluence by pulse	F_p	(J/m^2)	$F_p = 1$

Physical parameters of the gold nanoparticle			
Optical absorption section	A_{abs}	(nm^2)	$A_{abs} = 3623.8$
Diameter of the gold nanoparticle	D	(nm)	$D = 40$

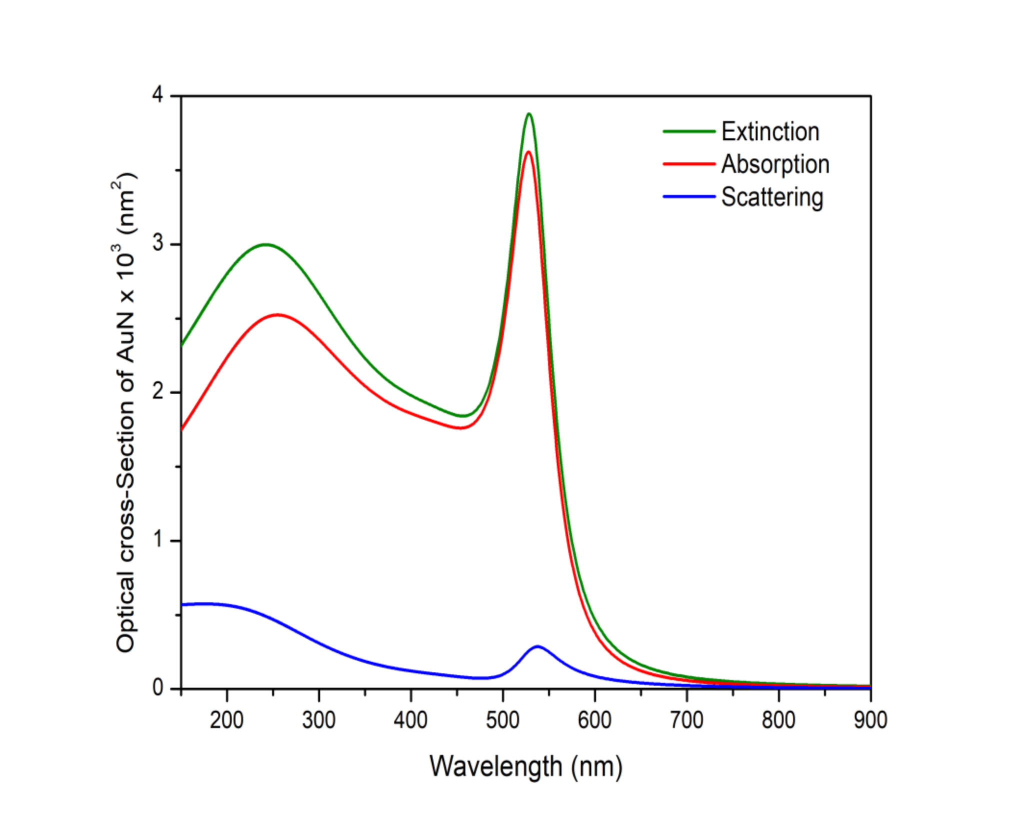


Figure 6: Cross sections of extinction, absorption, scattering as function of wavelength calculated by Mie code for AuN of diameter 40 nm.

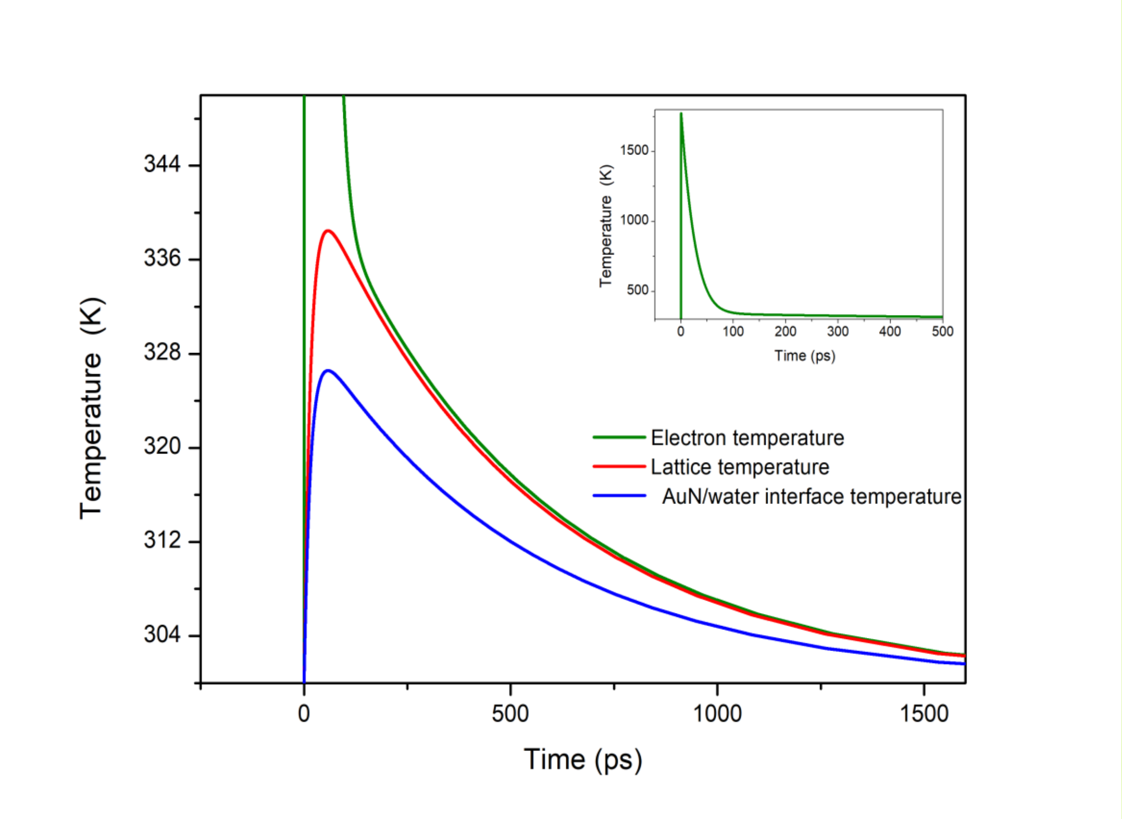
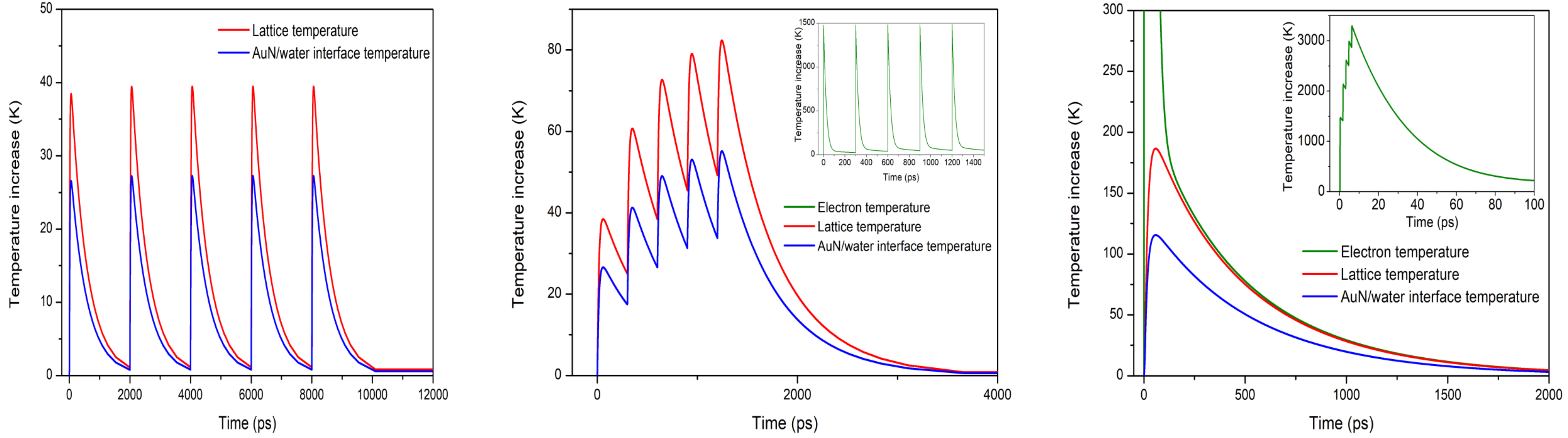


Figure 7: Temporal evolution of electron and lattice temperature of 40 nm-diameter AuN heated by femtosecond pulse and cooled in water. Duration time is 100 fs and fluence is 1 J/m2. In inset, temporal evolution of electron temperature.



(a) (b) (c)

Figure 9 : Time-temperature profile of AuN irradiated by multi-pulsed laser with a duration time 100 fs and fluence 1 J/m2, with a repetition rate of (a) 2 ns between pulses; (b) 300 ps between pulses; (c) 1.5 ps between pulses.

CONCLUSION AND PERSPECTIVES

- We studied the dynamics of thermal exchanges within a gold nanoparticle in a femtosecond regime.
- The pulsed signal is chosen as a single pulse and then a pulse burst.
- We used the TTM to describe the heat exchange process.
- The results founded show that the increasing of sub-pulses number with a separation time less than the thermal relaxation time can enhance the gold lattice temperature and the temperature at the AuN/water interface.
- The processes are ultrafast in the order of femtoseconds, picoseconds and nanoseconds.

Our future work focuses on the diffusion in the medium.

thank you for your

attention