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 nanoparticles that have extraordinary physical and chemical properties that allow them to be included in medicinal therapy and cancer treatment.

- The photonic energy emitted by a femtosecond laser is strongly absorbed by the gold nanoparticles injected into an individual's blood and then they become localized thermal 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 $\tau_p$ 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.

$$f(t) = \sum_{i=1}^{N} 2 \sqrt{\frac{\ln 2}{\pi}} e^{-4\ln(2) t^2/\tau_p^2}$$

$\tau_p$: 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.
Optical properties of gold NP

When a gold nanoparticle interacts with a light wave (laser) of wavelength \( \lambda \) (or frequency \( \omega \)), 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.

**Phase 1:** 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:

\[
\begin{align*}
C_e(T_e) \frac{dT_e(t)}{dt} &= -g(T_e - T_L) + S(t) \quad \text{(1)} \\
C_L(T_L) \frac{dT_L(t)}{dt} &= g(T_e - T_L) - Q_C
\end{align*}
\]

\[S(t) = \frac{1}{V_p} \frac{A_{abs} \times F_p}{\tau_p} \times f(t), \quad (2)\]

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

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

\(T_e(t)\) 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.
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, Te=TL=Tws =300 K).
- We simulated thermal dynamics by considering a single Gaussian profile multipulse.
### Simulation data

<table>
<thead>
<tr>
<th>Laser parameters</th>
<th>( \tau_p ) (ps)</th>
<th>( \tau_p = 100 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Pulse duration</td>
<td>( F_p ) (J/m(^2))</td>
<td>( F_p = 1 )</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Physical parameters of the gold nanoparticle</th>
<th>( A_{abs} ) (nm(^2))</th>
<th>( A_{abs} = 3623.8 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Optical absorption section</td>
<td>( D ) (nm)</td>
<td>( D = 40 )</td>
</tr>
<tr>
<td>Diameter of the gold nanoparticle</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
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.
Figure 9: Time-temperature profile of AuN irradiated by multi-pulsed laser with a duration time 100 fs and fluence 1 J/m$^2$, 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