Study of Thermal Conductivity of Nano-fluids Containing Gold Nanoparticles Using Moiré Deflectometry

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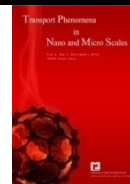**117** PUBLICATIONS   **865** CITATIONS

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Influence of interface thermal resistance on relaxation dynamics of metal-dielectric nanocomposite materials under ultrafast pulse laser excitation

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Abstract

Nanocomposite materials, including noble metal nanoparticles embedded in a dielectric host medium, are interesting because of their optical properties linked to surface plasmon resonance phenomena. For studding of nonlinear optical properties and/or energy transfer process, these materials may be excited by ultrashort pulse laser with a temporal width varying from some femtoseconds to some hundreds of picoseconds. Following of absorption of light energy by metal-dielectric nanocomposite material, metal nanoparticles are heated. Then, the thermal energy is transferred to the host medium through particle-dielectric interface. On the one hand, nonlinear optical properties of such materials depend on their thermal responses to laser pulse, and on the other hand different parameters, such as pulse laser and medium thermodynamic characterizes, govern on the thermal responses of medium to laser pulse. Here, influence of thermal resistance at particle-surrounding medium interface on thermal response of such material under ultrashort pulse laser excitation is investigated. For this, we used three temperature model based on energy exchange between different bodies of medium. The results show that the interface thermal resistance plays a crucial role on nanoparticle cooling dynamics, so that the relaxation characterized time increases by increasing of interface thermal resistance.

1. Introduction

In recent years, by miniaturizing of devices and novel applications in different domains of science and technology, heat transfer in micro- and nanoscale (low) dimension has been worthily investigated by many researchers [1,2]. In fact, nanocomposites materials have been proposed to use in different applications such as: cooling systems, thermo-optical and thermo-voltaic generators, imaging, sensing, biology, and medicine [3].Indeed, it has been shown that the suspended nanoparticles may increase

thermal conductivity of the base liquid [4,5].In addition, light-heat conversion in low dimensions has been opened the new applications [6,7]. Even recently, it has been shown that the thermal analogues of electrical devices, as diode and transistor, may be designed using the heat transfer principals in low dimension [1,2]. host medium, have been worthily studied thanks to their attractive optical properties linked to the Surface Plasmon Resonance (SPR) phenomena [8,9]. This is related to the coherence oscillation of metal nanoparticle free electrons under electrical field of light and lead to increasing of optical absorption around a frequency, known as SPR frequency. So, these materials have been proposed for

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Nomenclature			Greek Symbols	
A	num power absorbed per metal volume unit (W m-3)		γ	Electron heat capacity coefficient (J m^{-3})
C	Specific heat capacity (J K-1 m-3)		**Subscripts**	
F	Heat power flux density (W m-2)		e	electron
G	Electron-phonon coupling constant (W m-3 K-1)		l	lattice
g	Thermal conductivity at interface (W m-2 k-1)		m	matrix
K	Heat conductivity (W m-2 k-1)			
Pvol(t)	Instantaneous power absorbed per metal volume unit (W m-3)			
T	Temperature (K)			
t	Time (s)			
v	Volume (m^{-3})			

numerous applications such as photonic devices, molecular sensing, biological cell imaging, or photothermal therapy [3,10,11]. In many of these applications, the materials are exposed to the light. Particularly, to study of their nonlinear optical properties, a pulsed laser with temporal bandwidth varying from some tens of femtoseconds to some hundreds of picoseconds is applied [12,13]. Consecutively, the optical properties of material may be modified by Thermal phenomena of different origins [13-16]. The laser pulse energy is absorbed partially by free electrons of metal nanoparticles via electron-photon interaction. Due to electron-electron collision, this energy is redistributed in metal free electron gas. So, the free electron distribution may be described by Fermi-Dirac distribution [12-13]. Depending on the laser pulse and metal characteristics, these processes could take for some hundreds of femtoseconds and known as a thermal regime [13]. Due to electron-phonon coupling, the energy is then transferred to the nanoparticle metal lattice. It should be mentioned that as specific thermal capacity of lattice is about two orders of magnitude larger than that electron gas, the electron gas temperature may be increased to some thousands of Kelvin, while the lattice temperature rises just some Kelvins. At last, the energy is transferred to host dielectric medium through the nanoparticle-dielectric interface. On the one hand, the optical properties of medium under the pulse laser excitation depend on thermal relaxation of materials and on the other hand thermal relaxation depends on different parameters such as pulse laser characterizations, thermodynamics properties of nanoparticle and its environment, nanoparticle shape and interface thermal resistance

[14]. This earlier, known as Kapitza resistivity, is due to the contact between two materials and provokes a temperature jump at interface when thermal energy flux passes through interface. So this effect plays a crucial role in thermal dynamics of embedded nanoparticles under pulsed laser excitation [17-19].

To study influence of thermal resistance on thermal relaxation of metal nanoparticle embedded in a dielectric host medium, we used three temperature model which is presented in following section.

2.Mathematical modeling :
2.1 Three Temperature Model (TTM)

TTM may be used to determine the temperature dynamics of nanocomposite materials, including metal nanoparticle dispersed in a dielectric host medium under laser pulse excitation. This model is based on energy exchange between different components of material, i.e. electron gas and lattice of metal nanoparticle and its surrounding medium [12, 20]. In present model, the a thermal regime is disregarded. Thus, the electron temperature T_e may be defined instantaneously as a function of time. In addition, since the nanoparticle size, in order of some nanometers, is very smaller than the laser wavelength, whole of the particle will be exposed by the same electrical field intensity. So, all of particle volume is heated simultaneously and therefore the electron and phonon diffusion in particle may be ignored. Two opposite terms govern on temporal evolution of electron temperature: it increases by absorption of

laser energy and it decreases because of energy transferred to metal lattice via electron-phonon coupling. So we have:

$$C_e \frac{\partial T_e}{\partial t} = -G(T_e - T_l) + P_{vol}(t) \qquad (1)$$

where T_l, G and C_e are lattice temperature, electron-phonon coupling constant and electron bath heat capacity respectively. This earlier may be given as $C_e = \gamma_e T_e$ where γ_e is a constant. $P_{vol}(t)$ is instantaneous power absorbed per metal volume unit and depends on the laser and material characterizations. It should be mentioned that $P_{vol}(t)$ is depend on the laser characterizes as well as the optical properties of the material. The lattice temperature is increased due to the energy transferred from free electron and it is decreased because of energy transferred to the nanoparticle host medium. So one can write:

$$C_l \frac{\partial T_l}{\partial t} = G(T_e - T_l) - \frac{H(t)}{V_p} \qquad (2)$$

Where V_p is the volume of particle and $H(t)$ is the heat power flux transferred to the nanoparticle host medium and may be written as follows:

$$H(t) = \int_S \mathbf{F} . \mathbf{ds} \qquad (3)$$

where F is density of heat power flux at surface of nanoparticle and may be related to the thermal conductivity at particle-medium interface g and temperature jump at surface of the particle ΔT using following equation [21]:

$$\mathbf{F} = g\,\Delta T \qquad (4)$$

At last, when characteristic size of material is very larger in compare to the heat carrier mean free path, energy transfer in the medium may be written using classical diffusion equation given by Fourier low [22]:

$$C_m \frac{\partial T_m(\mathbf{r},t)}{\partial t} = -\nabla . \mathbf{F}_m(\mathbf{r},t) \qquad (5)$$

where C_m and $T_m(\mathbf{r},t)$ denote heat capacity and the temperature of the nanoparticle host medium at point r and time t respectively.

$\mathbf{F}_m(\mathbf{r},t)$ represents the instantaneous density of the heat power flux at point $\mathbf{r}$. This earlier could be related to temperature gradient in the medium $\nabla T_m(\mathbf{r},t)$ as:

$$\mathbf{F}_m(\mathbf{r},t) = -K_m \nabla T_m(\mathbf{r},t) \qquad (6)$$

2.2 Application for gold nanoparticle embedded in silica

The present model is applied to determine the temperature evaluation of electron gas and metal lattice of a gold nanoparticle embedded in silica as well as temperature evolution at each point of this earlier under the ultrashort pulse laser excitation. For this, the coupled equations 1 to 4 should be solved and as any analytical solution was not founded, we used a numerical method based on the finite element method. Moreover, as temporal profile of laser pulse intensity is a Gaussian, instantaneous power absorbed per metal volume unit is also considered as a Gaussian of $P_{vol} = A \exp\left(-B\left(t - t_0\right)^2\right)$ where A is related to laser pulse characterizes and optical absorption of the medium and B is related to the temporal bandwidth of laser pulse. Here, A and B are chosen the same values that used in reference [12]. On the other hand, thermodynamics parameter values were considered as their bulk values [22]:

$$C_l = 2.49 \times 10^6 \, Jm^{-3} K^{-1}, \, G = 3 \times 10^{16} \, wm^{-3} K^{-1},$$

$$K_m = 1.378 \, wm^{-1} K^{-1}, \, D_m = 7.49 \times 10^{-7} \, m^2 s^{-1}$$

$$\gamma_e = 66 \, Jm^{-3} K^{-2}.$$

Let us to mention that thermodynamics parameter values in low dimension materials may be different from those of their bulk values. Particularly, it has been shown a particle size dependence of particle-medium interface thermal conductivity [21]. However, such dependences may be included in the present model.

3. Results and discussions

Let us firstly to evaluate the influence of particle-medium interface thermal conductivity on electron and lattice temperature dynamics of a gold nanoparticle embedded in silica under a femtosecond pulse laser. For this are compared electron and lattice temperature arise dynamics of a nanoparticle, $\Delta T_e(t)$ and $\Delta T_l(t)$, by considering an interface thermal resistivity corresponding to $g = 10^8$ Wm^{-2}K^{-1} and those of a nanoparticle without any interface thermal resistivity ($g = \infty$). This earlier is corresponding to a perfect thermal contact between particle and its surrounding medium. The results are shown in figure 1 in which $\Delta T_e(t)$ and $\Delta T_l(t)$ are presented in logarithm scale. Inset in this figure represents $\Delta T_e(t)$ in linear scale. As we can see, there is not any interface thermal resistance effect on the electron temperature dynamic for some first picoseconds but after this time period we observe that the electron temperature dynamics is affected by the thermal interface resistance: the more interface thermal resistance, the longer relaxation time characterization. To understand these behaviors, it should mentioned that as electron-phonon relaxation time characterize is some picoseconds, absorbed energy by free electrons is not transferred to nanoparticle lattice effectively during these first picoseconds. Consequently the absorbed energy is stoked in free electron gas and therefore $\Delta T_e(t)$ is independent from particle shape, surrounding medium and spatially from interface thermal resistivity. During these times, $P_{\text{vol}} \approx 0$ and on the other hand $\Delta T_l(t)$ is negligible comparing to $\Delta T_e(t)$.
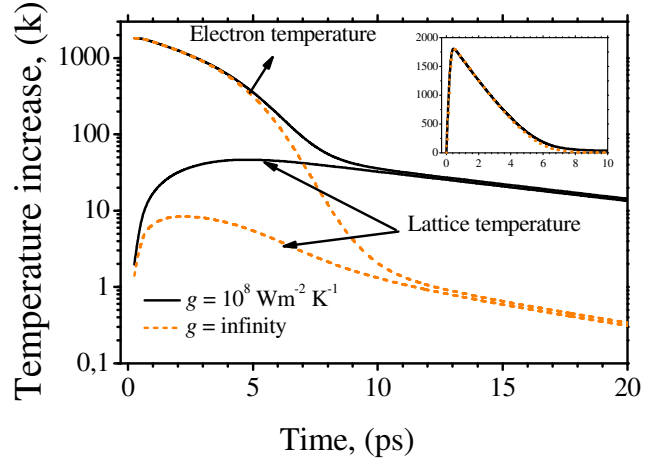

Fig.1. Electron and lattice temperature increase of a gold nanoparticle of 1.3 nm of radius embedded in silicate medium under ultrashort laser pulse excitation in logarithm scale. Temporal bandwidth of laser pulse is considered 110 femtoseconds. Solid and Dash curves are corresponding to $g = 10^8$ Wm^{-2}K^{-1} and $g = 0$ respectively. Inset presents electron temperature in linear scale

Hence, one can obtain simply electron temperature dynamics from equation 1:

$$T_e(t) = T_{e,\max} - \frac{G}{\gamma} t \qquad (7)$$

where $T_{e,\max}$ is maximum value of electron temperature which may be approximated as following:

$$T_{e,\max} = \left(T_0^2 + \frac{2A}{\gamma} \sqrt{\frac{\pi}{B}} \right)^{1/2} \qquad (8)$$

Electron relaxation characterize time during this period of time, defined as time in which T_e decreases to $\frac{1}{2} T_{e,\max}$, may be evaluated as $\tau_1 = \frac{\gamma T_{e,\max}}{2G}$. For the values considered here τ_1 is about 2.2 ps which is a very good agreement with the calculated value (see inset in figure 1).

Due to electron-phonon interaction, the absorbed energy by free electron gas is transferred to nanoparticle metal lattice. This may last for some

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picoseconds. After this time electron and lattice attain a thermodynamic equilibrium.So,electron and lattice temperature evolution are controlled by $H(t)$ that depends directly to the interface thermal resistance. This may be observed in figure 2a that presents lattice temperature dynamics for different values of *g*, varying from zero to infinity. These values correspond to an isolate particle and perfect thermal contact at particle-surrounding medium interface respectively.

As we can see in figure 2a, $T_l(t)$ increases to a maximum value then it decay to ambient temperature. The maximum value of $T_l(t)$, $T_{l,max}$, as well as the time for which $T_l(t)$ reaches to its maximum value depends to *g*. In this case, with increasing of *g*, $T_{l,max}$ decrease and $T_l(t)$ attain to its maximum at shorter time. In addition, the relaxation time characteristic depends on *g*. These two earlier effects may be observed better in figure 2b that presents normalized lattice temperature dynamics in logarithm scale for different values of *g*. To understand these behaviors, it should be mentioned that two competition terms govern on lattice temperature dynamics (see equation2). First one denotes the absorbed energy from free electron gas of nanoparticle. This term independent to *g* for some first picoseconds. But the second one, that represents the energy transferred to the host medium, depends directly to thermal resistance at nanoparticle-medium interface: the higher interface thermal resistance, the slower is heat transfer rate to nanoparticle environment.
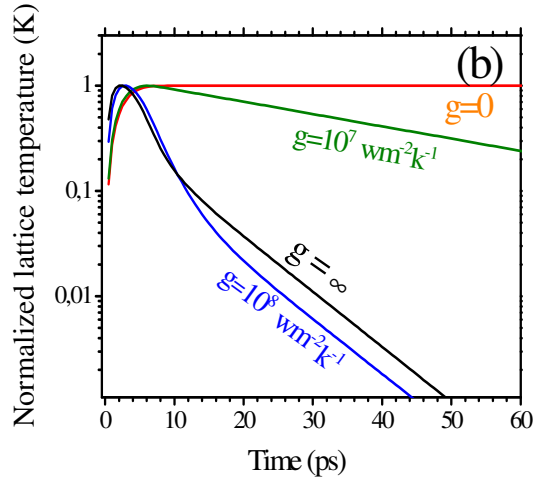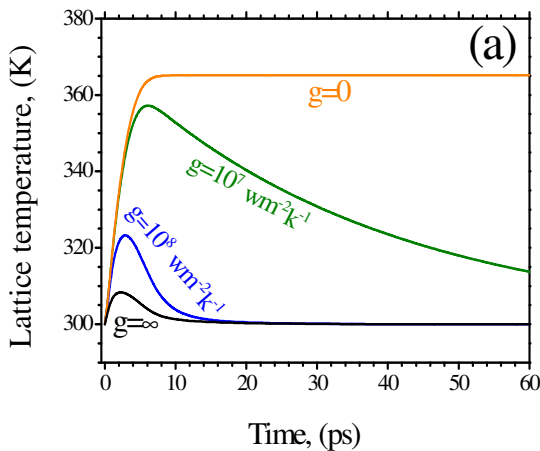

Fig.2. Lattice temperature of a gold nanoparticle (a) and normalized lattice temperature in logarithm scale (b) for different values of thermal conductance at nanoparticle-host medium interface, varying from *g* = 0 to infinite.

Therefore by increasing in interface thermal resistance, accumulated heat energy in the nanoparticle will be increased. Consequently, T_l increases and it reaches to its maximum value at later time. On the other hand, we can observe two kind of relaxation characterized times in T_l for high value of g (see figure 2b), but just one kind of relaxation characterized time in T_l may be observed for weak value of *g*. It can be mentioned that lattice cooling may be controlled by two physical parameters: *g* and temperature gradient at interface. For a high value of g, during short time periods, the particle cooling dynamics is controlled by the temperature gradient at the surface of the nanoparticle, but after some first ps, it is controlled by *g*. As we can see in figure 2b, during these short times, T_l decays exponentially depending to *g*. For the values considered here, the relaxation characterized time vary from 8 ps to infinity when *g* vary from infinity to zero.

4.Conclusion

In this research, influence of nanoparticle-host medium interface thermal resistance on the thermal dynamics of a gold nanoparticle embedded in a dielectric medium under an ultrashort laser pulse excitation was determined using TTM. During some first picoseconds, electron temperature dynamics of nanoparticle is independent to interface thermal

resistance. But after some picoseconds, it depends to thermal resistance at nanoparticle-medium interface. On the other hand, it has been observed that lattice temperature dynamics is affected by interface thermal resistance.

These results are expected to analyses of ultrashort pomp-probe spectroscopy experiments for determining of nonlinear optical properties or investigation of energy transfer process in embedded nanoparticles. In such experiments, temporal optical variation, induced by pomp laser beam, is measured using probe beam with different delay times respect to pomp one.

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