Thermomechanical action of ultrashort laser pulses on metallic nanostructures

Oleg Romanov[1], Gennady Romanov[2]

[1] Belarusian State University, Minsk, Belarus

[2] A.V. Luikov Heat and Mass Transfer Institute, National Academy of Sciences of Belarus, Minsk, Belarus

Introduction

Excitation of acoustic vibrations in spherical metallic nanoparticles

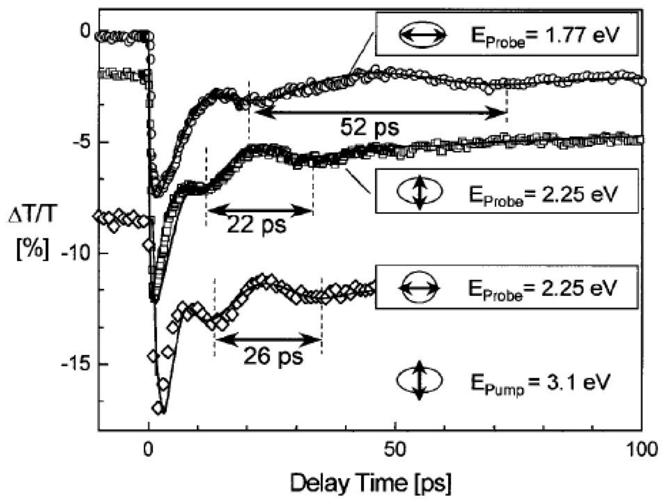


FIG. 2. Differential transmission transients (upper curves: ellipsoidal particles; lowest curve: spherical particles; the transients are vertically offset for clarity). The light polarizations and photon energies of the pump and probe pulses are indicated. Solid lines: fits to the data as explained in part (iv) of the text.

pump – probe spectroscopy

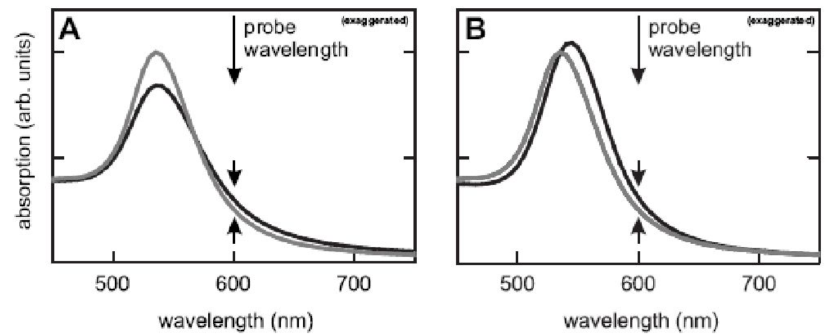


Figure 1.11: Sketch of the effect of the electronic temperature rise (A) and the lattice expansion (B) on the absorption spectrum of a gold nanoparticle. The grey lines are the absorption spectrum of an unperturbed or cold nanoparticle. The black lines give the absorption spectrum of an excited gold nanoparticle. The heating of the electrons broadens the spectrum, while the heating of the lattice causes a red shift.

$$T_{R_0} = 2R_0/u_0 \approx \frac{10^{-6}\,cm}{10^5\,cm/s} \approx 10\,ps$$

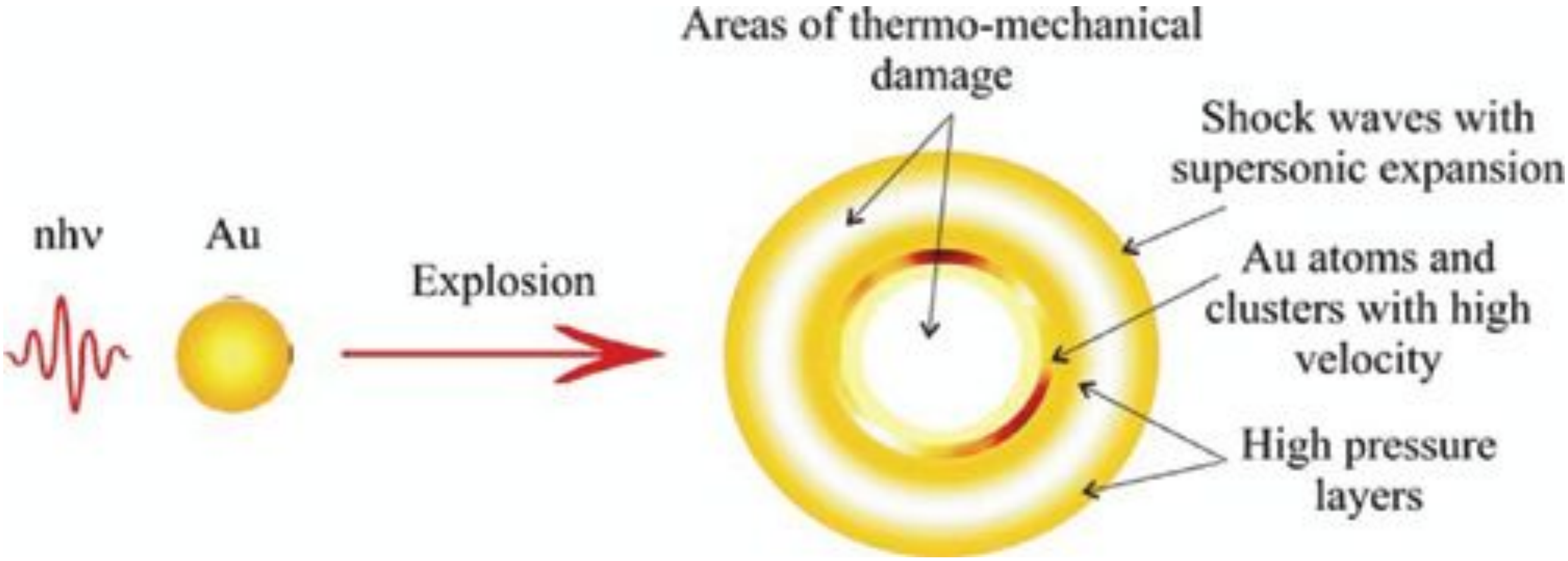
Damping oscillations:

$$\frac{d^2}{dt^2}\Delta x + 2\rho\frac{d}{dt}\Delta x + \omega_0^2\Delta x = A\sigma/m\,, \qquad (1)$$

M. Perner, S. Gresillon, J. März, G. von Plessen, J. Feldmann // Phys. Rev. Lett. 2000. V.85. P.792.

Introduction

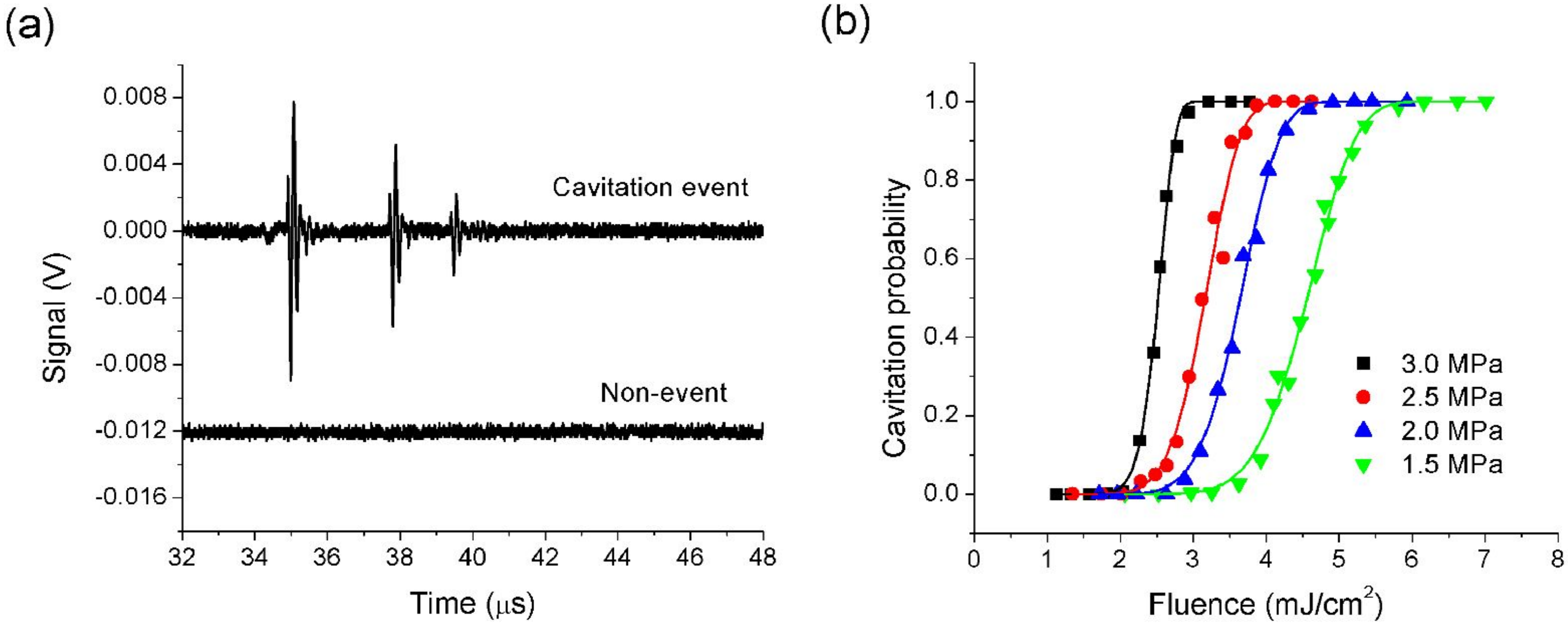
Laser-induced explosion of gold nanoparticles: potential role for nanophotothermolysis of cancer



R. Letfullin, Ch. Joenathan, Th. George, V. Zharov // Nanomedicine, 2006, V.1. P.473.

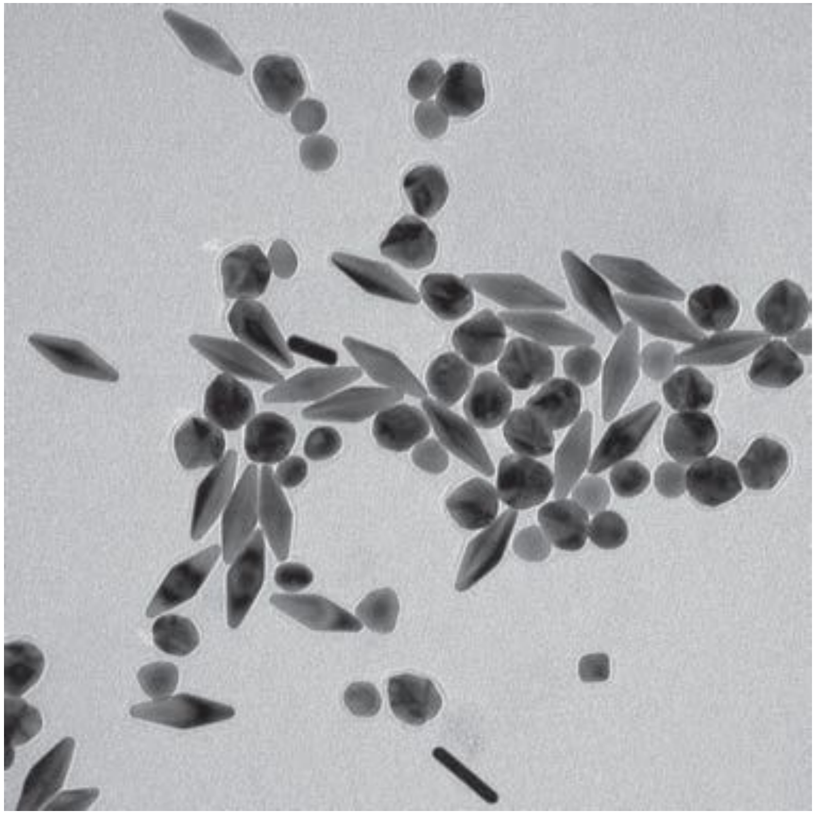
Cavitation phenomena around nanoparticles

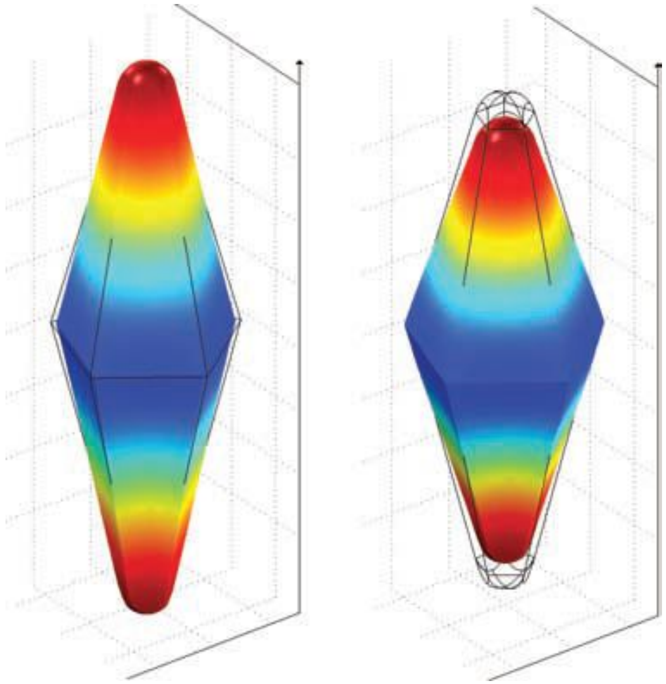
Gold nanoparticle targeted photoacoustic cavitation for potential deep tissue imaging and therapy / Hengyi Ju, Ronald A. Roy, and Todd W. Murray **//** BIOMEDICAL OPTICS EXPRESS 2013 / Vol. 4, No. 1 P. 66



(a) Acoustic signals from a photoacoustic cavitation event and a non-event around gold nanospheres (2.2×10^8 nanoparticles/ml) at a peak negative HIFU pressure of 1.5 MPa and a laser fluence of 4.8 mJ/cm2. (b) Cavitation probability as a function of laser fluence around gold nanospheres (2.2 × 108 nanoparticles/ml) at peak negative pressures of 1.5, 2.0, 2.5 and 3.0 MPa.

Excitation of acoustic vibrations in nonspherical metallic nanoparticles

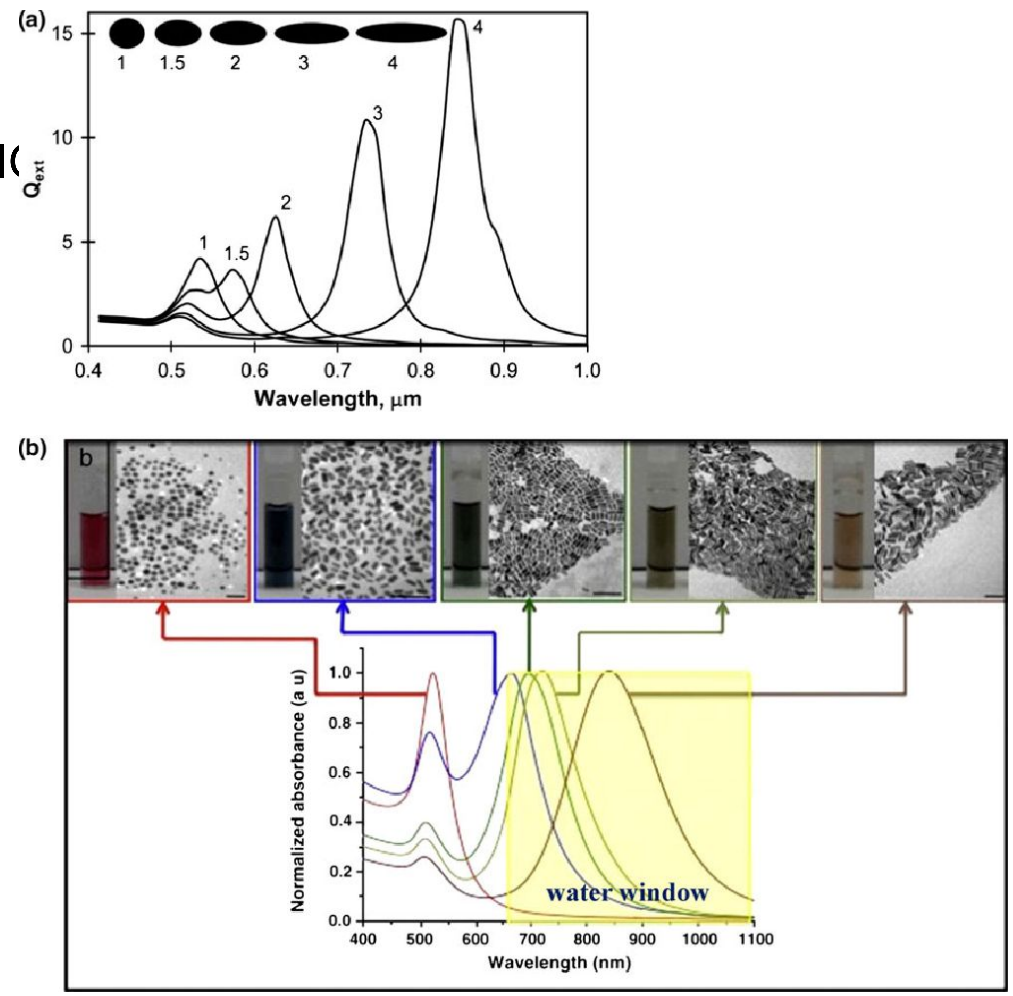




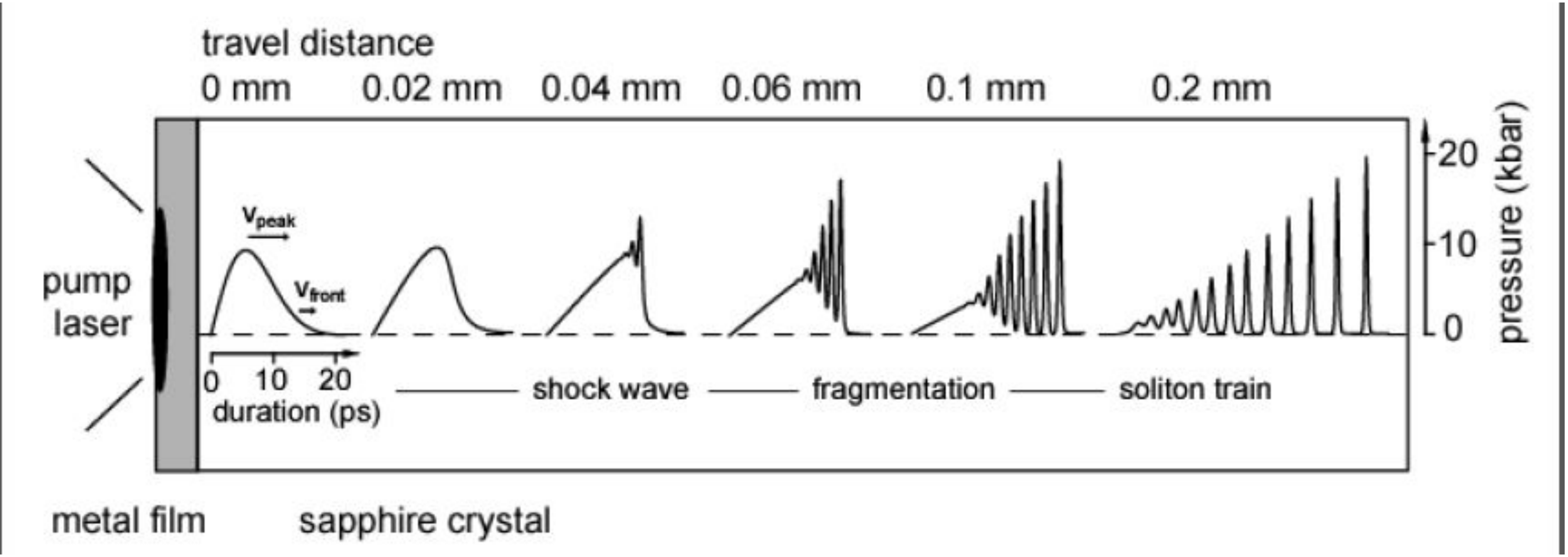
Damping of acoustic vibrations in gold nanoparticles. Matthew Pelton, John E. Sader, Julien Burgin, Mingzhao Liu, Philippe Guyot-Sionnest and David Gosztola // NATURE NANOTECHNOLOGY VOL 4 2009 P.492

Excitation of acoustic vibrations in nonspherical metallic nanoparticles

Photothermal Cancer Therapy and Imaging Based on Gold Nanorods
WON IL CHOI, ABHISHEK SAHU, YOUNG HA KIM, and GIYOONG TAE // Annals of Biomedical Engineering (2011)
DOI: 10.1007/s10439-011-0388-0

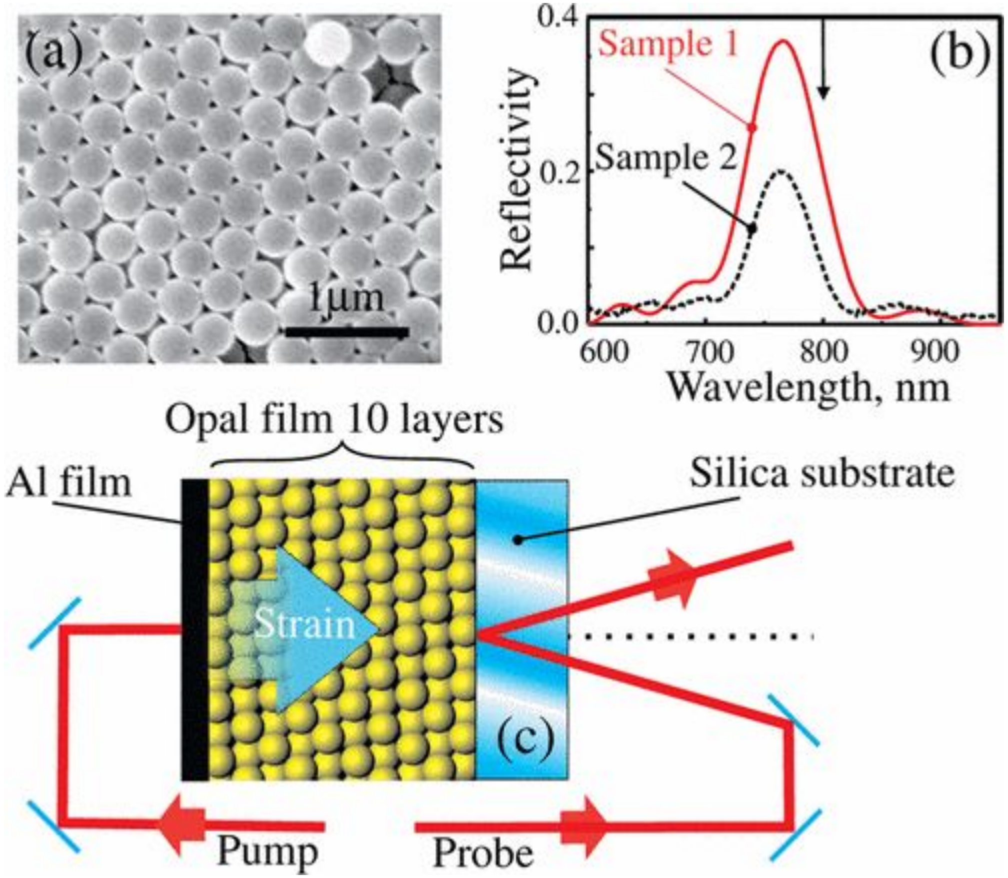


Excitation of shock waves under absorption of laser radiation in metallic films



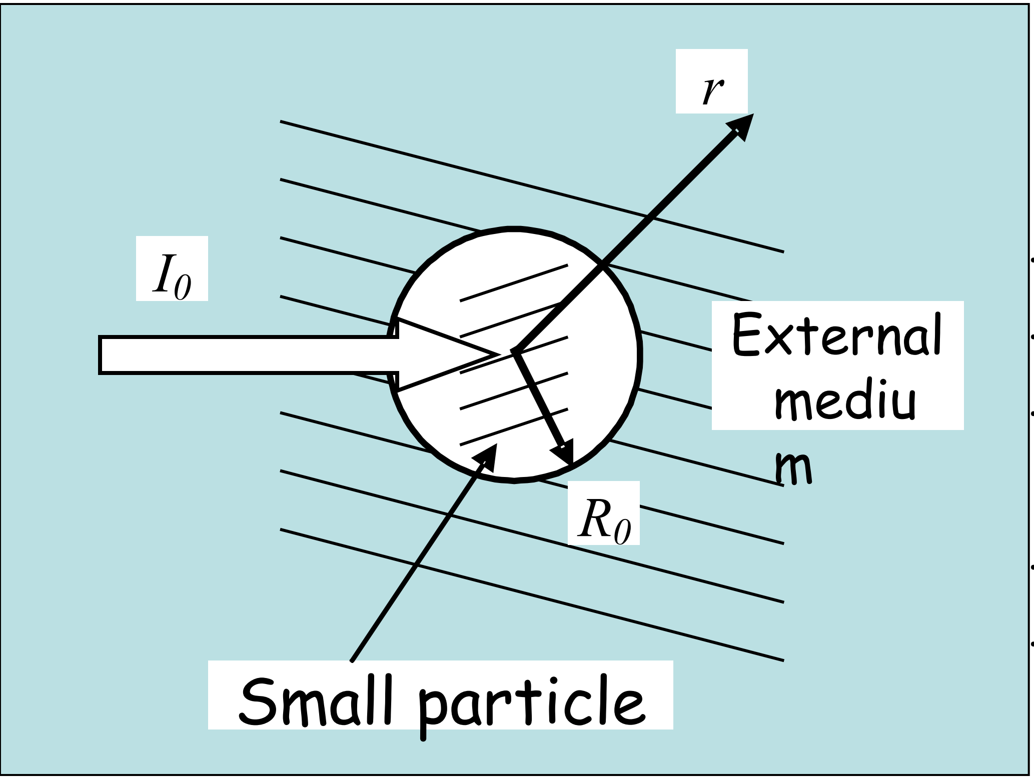
Ultrashort strain solitons in sapphire and ruby / Otto Muskens et.al.

Hypersonic Modulation of Light in Three-Dimensional Photonic and Phononic Band-Gap Materials



A. V. Akimov, Y. Tanaka, A. B. Pevtsov, S. F. Kaplan, V. G. Golubev, S. Tamura, D. R. Yakovlev, and M. Bayer // Phys. Rev. Lett. 101, 033902

Theoretical model



Main stages of thermooptical excitation of acoustic pulse:

- -absorption of laser pulse energy;
- -local heating;
- -local pressure increasing;
- -expansion due to gradient of pressure;
- -formation of acoustic pulse;
- -relaxation process.

The Lagrange equations for the one-dimensional motion of a continuous medium have the following form [1]:

$$V = V_0 \left(\frac{R}{r}\right)^{\alpha-1} \frac{\partial R}{\partial r}$$ – continuity equation

$$\frac{\partial u}{\partial t} = -V_0 \left(\frac{R}{r}\right)^{\alpha-1} \frac{\partial P}{\partial r}$$ – motion equation

$$\frac{\partial R}{\partial t} = u$$ – equation of the changing of Euler coordinate R

$$P = \rho_0 c_0^2 \left(1 - \frac{V}{V_0}\right) + \Gamma \frac{C(T - T_0)}{V}$$ – Mie-Grünheisen state equation

$$\rho C \frac{\partial T}{\partial t} = k \Delta T + Q_s$$ – heat transfer equation

α=1 – plane
α=2 – cylindrical
α=3 – spherical geometry

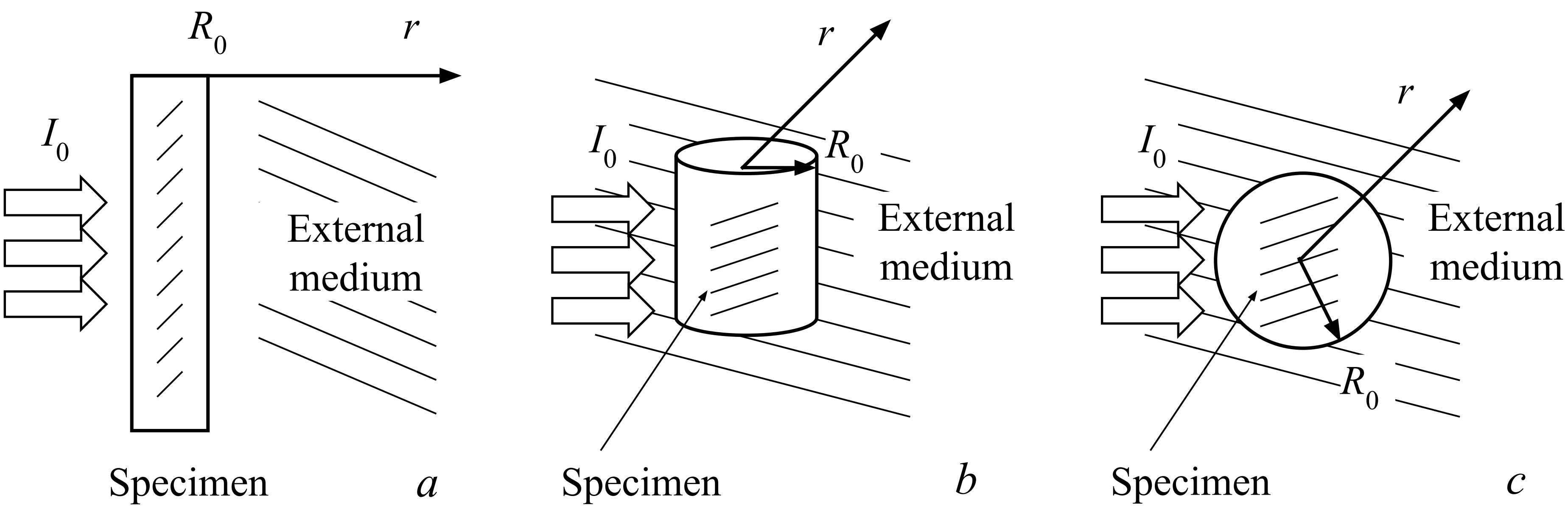
→ P (r,t), u (r,t), ρ (r,t), T (r,t)

[1] O.G. Romanov, G.I. Zheltov, G.S. Romanov. Numerical modeling of thermomechanical processes in absorption of laser radiation in spatially inhomogeneous media // Journal of Engineering Physics and Thermophysics, 2011. Vol. 84, No. 4, P.772-780.

Theoretical model

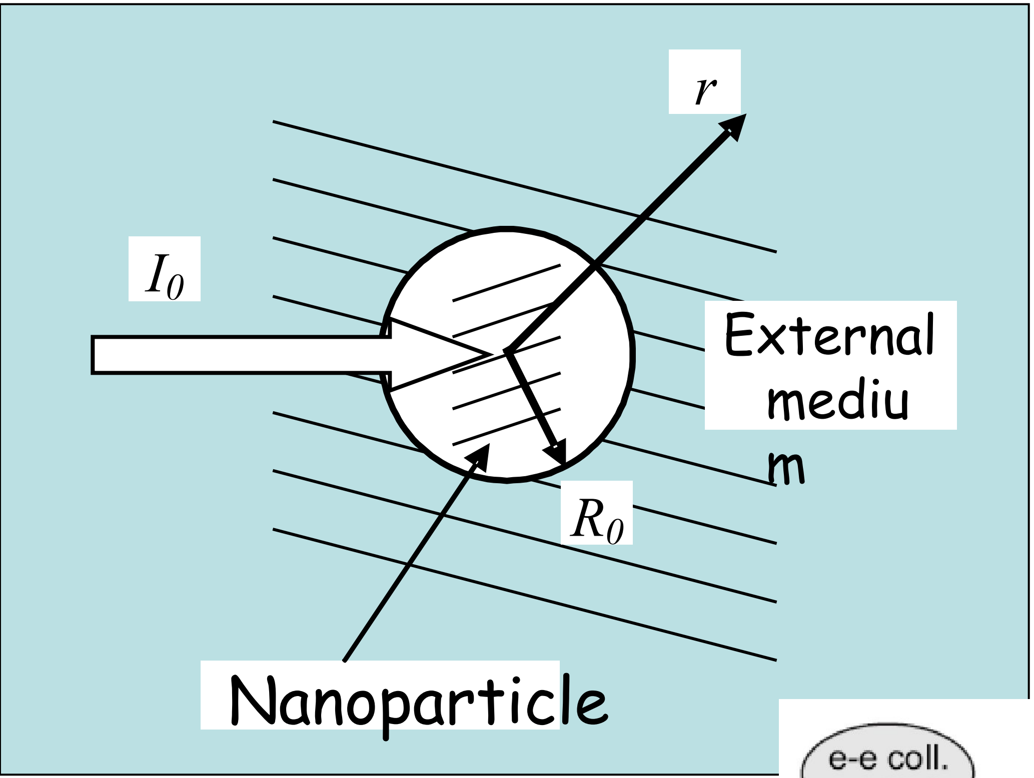
Peculiarities of the problem:

- size of metallic structures (10-100 nm);
- pulse duration (100 fs).



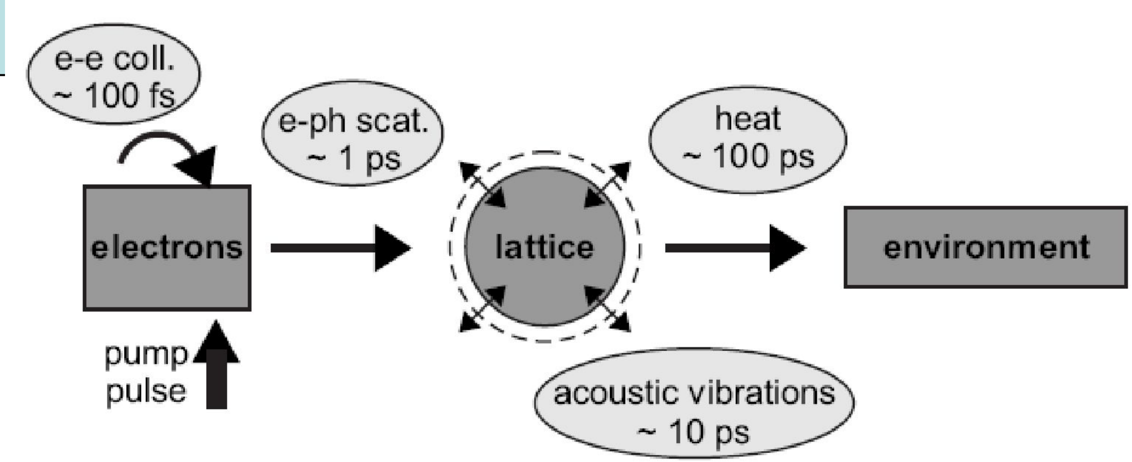
Scheme of radiation–medium interaction in the plane (a), cylindrical (b), and spherical (c) geometries.

Theoretical model



- particle size (10-100nm);
- pulse duration (100fs);

Fast dynamics in small area



Theoretical model

The heating of metals with ultra short laser pulses is described by a two-temperature model for an electron gas and an ionic lattice:

heat source function

$$\rho_e C_e \frac{\partial T_e}{\partial t} = k_T^e \frac{1}{r^2} \frac{\partial}{\partial r}\left(r^2 \frac{\partial T_e}{\partial r} \right) + Q_S - \gamma\left(T_e - T_i\right)$$

$$\rho_i C_i \frac{\partial T_i}{\partial t} = \gamma\left(T_e - T_i\right)$$

electron-phonon relaxation

S.I.Anisimov, Ya.A. Imas, G.S. Romanov, and Yu.V. Khodyko.
The Effect of High Power Radiation onto Metals, 1970 (in Russian).

Theoretical model

Mie–Grünheisen state equation for metallic nanoparticle:

$$P = \rho_{i0} u_0^2 \left(1 - \frac{V_i}{V_{i0}} \right) + \Gamma_i \frac{C_i \left(T_i - T_0 \right)}{V_i} + \Gamma_e \frac{C_e \left(T_e - T_0 \right)}{V_e}$$

Mie–Grünheisen state equation for environment:

$$P = \rho_0 u_l^2 \left(1 - \frac{V}{V_0} \right) + \Gamma \frac{C \left(T - T_0 \right)}{V}$$

Numerical model

Lagrange equations [2]:

[2] R.D. Richtmayer, and K.W. Morton, *Difference Methods for Initial Value Problems*, 1967.

$$V_{j+1/2}^{n+1} = V_0 \frac{\left(R_{j+1}^{n+1}\right)^{\alpha} - \left(R_j^{n+1}\right)^{\alpha}}{\left(r_{j+1}\right)^{\alpha} - \left(r_j\right)^{\alpha}}$$

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} = -V_0 \frac{(\delta p)_j^n + (\delta q)_j^n}{\Delta r} \left(\frac{R_j^n}{r_j}\right)^{\alpha-1}$$

$$\frac{R_j^{n+1} - R_j^n}{\Delta t} = u_j^{n+1}$$

Artificial viscosity

$$(\delta q)_j^n = q_{j+1/2}^n - q_{j-1/2}^n$$

$$q_{j+1/2}^n = \begin{cases} \frac{2a^2}{V_{j+1/2}^n + V_{j+1/2}^{n-1}} \left[(\delta u)_{j+1/2}^n\right]^2, (\delta u)_{j+1/2}^n < 0; \\ 0, (\delta u)_{j+1/2}^n \geq 0; \end{cases}$$

$$(\delta u)_{j+1/2}^n = u_{j+1}^n - u_j^n$$

$$\Delta t = t^{n+1} - t^n$$

$$\Delta r = r_{j+1} - r_j$$

$$(\delta p)_j^n = P_{j+1/2}^n - P_{j-1/2}^n$$

Numerical model

Heat transfer equation [3]:

$$\frac{T_j^{n+1}-T_j^{n-1}}{2\Delta t}=\frac{V_j^n}{C_V}k_T\left(\frac{\alpha-1}{r_j}\frac{T_{j+1}^n-T_{j-1}^n}{2\Delta r}+\frac{T_{j+1}^n-2T_j^n+T_{j-1}^n}{(\Delta r)^2}\right)+\frac{V_j^n}{C_V}(Q_S)_j^n.$$

$$T_j^n=\tfrac{1}{2}\left(T_j^{n+1}+T_j^{n-1}\right)$$

[3] V.K. Saul’ev, Parabolic Equations Integration by Grid Method, 1960 (in Russian).

Plane geometry

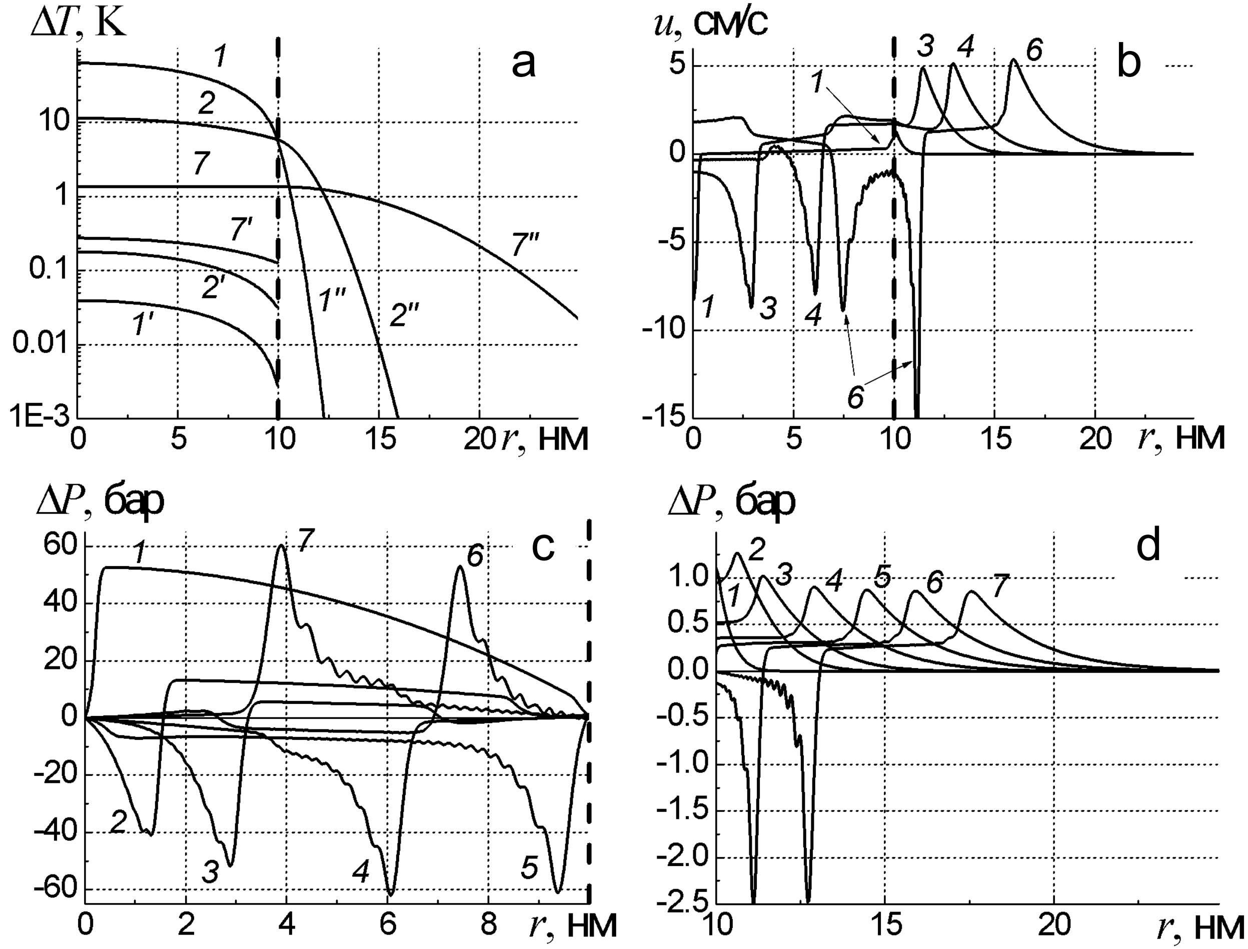
α=1

$$I_0 = 10^{10} W / cm^2$$

$$\tau_p = 100 fs$$

$$R_0 \approx 10nm$$

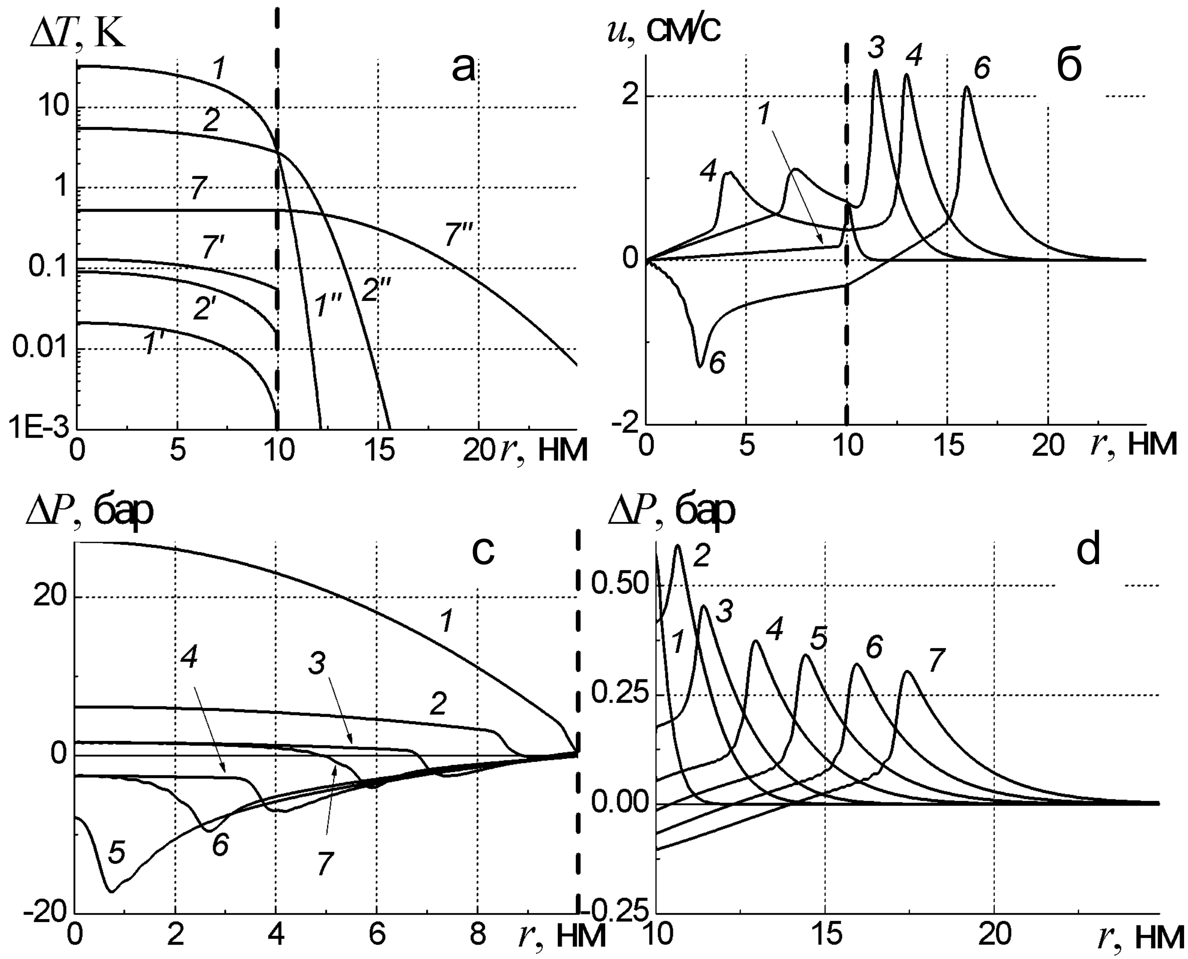
$$\kappa = 10^5 cm^{-1}$$



Space distributions of temperature (*a*), velocity (*b*) and pressure (*c*, *d*) in different time moments.
1 – 100 fs, 2 – 500 fs, 3 – 1 ps, 4 – 2 ps, 5 – 3 ps, 6 – 4 ps, 7 – 5 ps

Results and discussion

Cylindrical geometry
α=2



$$I_0 = 10^{10} W / cm^2$$

$$\tau_p = 100 fs$$

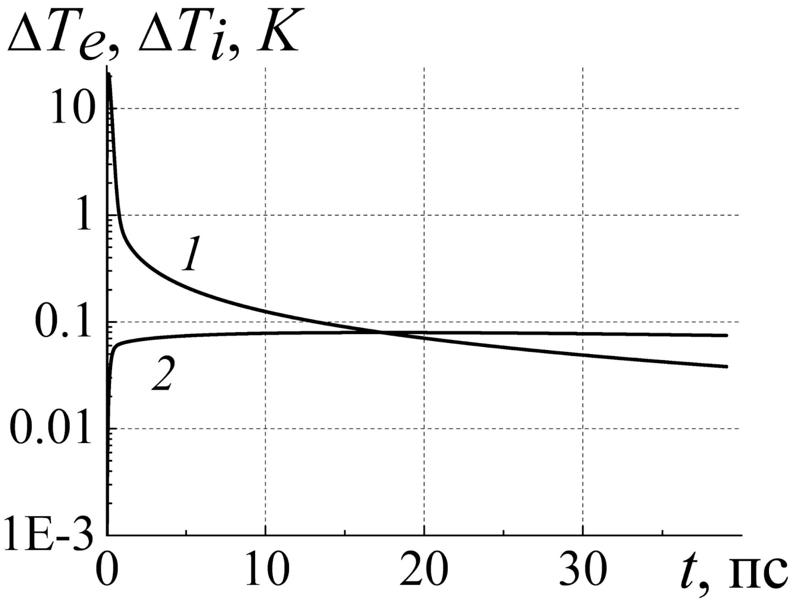
$$R_0 \sim 10 nm$$

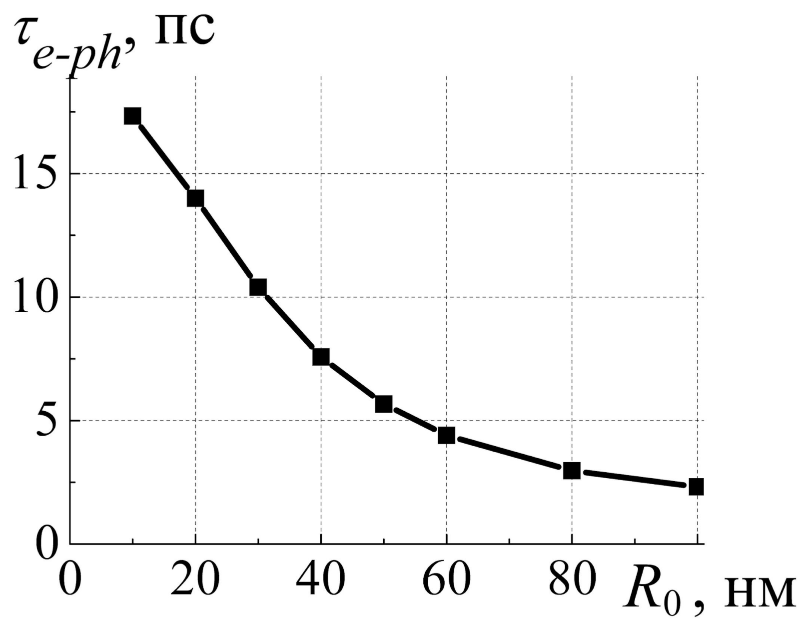
$$\kappa = 10^5 cm^{-1}$$

Space distributions of temperature (*a*), velocity (*b*) and pressure (*c*, *d*) in different time moments.
1 – 100 fs, 2 – 500 fs, 3 – 1 ps, 4 – 2 ps, 5 – 3 ps, 6 – 4 ps, 7 – 5 ps

Results and discussion

Spherical geometry: gold nanoparticle in water





Time dependences of temperature in the centre of gold nanoparticle

$I_0 = 10^{10} W / cm^2 \quad \tau_p = 100\, fs \quad R_0 \approx 10 nm \quad \kappa = 10^5 cm^{-1}$

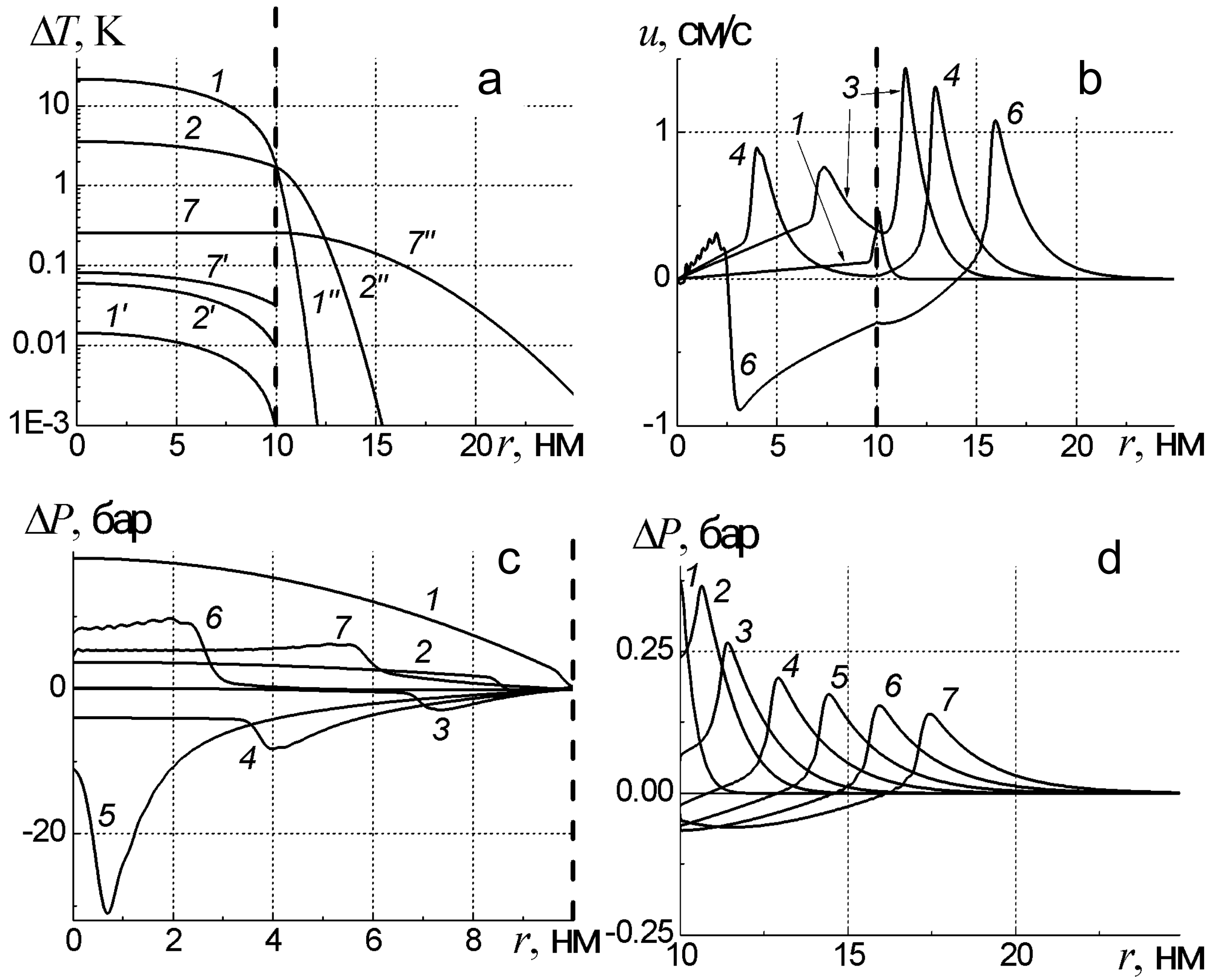
Сферическая геометрия
α=3

$$I_0 = 10^{10} W / cm^2$$

$$\tau_p = 100 fs$$

$$R_0 \approx 10nm$$

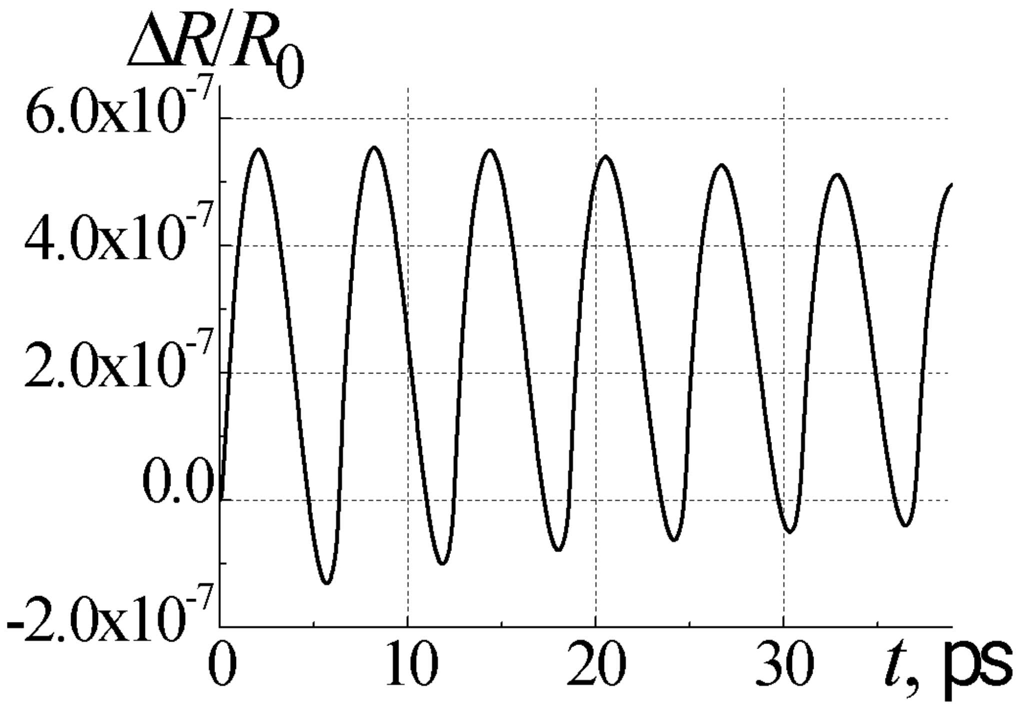
$$\kappa = 10^5 cm^{-1}$$

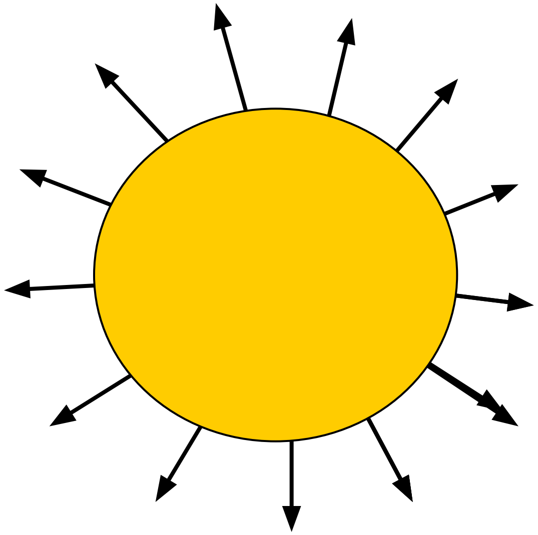


Space distributions of temperature (*a*), velocity (*b*) and pressure (*c*, *d*) in different time moments.
1 – 100 fs, 2 – 500 fs, 3 – 1 ps, 4 – 2 ps, 5 – 3 ps, 6 – 4 ps, 7 – 5 ps

Results and discussion

Spherical geometry: gold nanoparticle in water



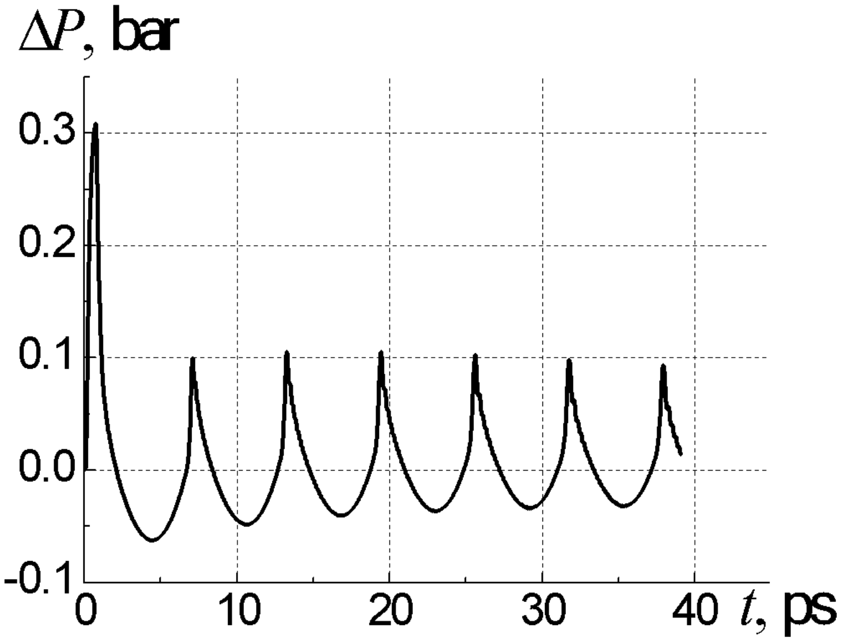


$$T_{R_0} = 2R_0/u_0 = 6.2\,ps$$

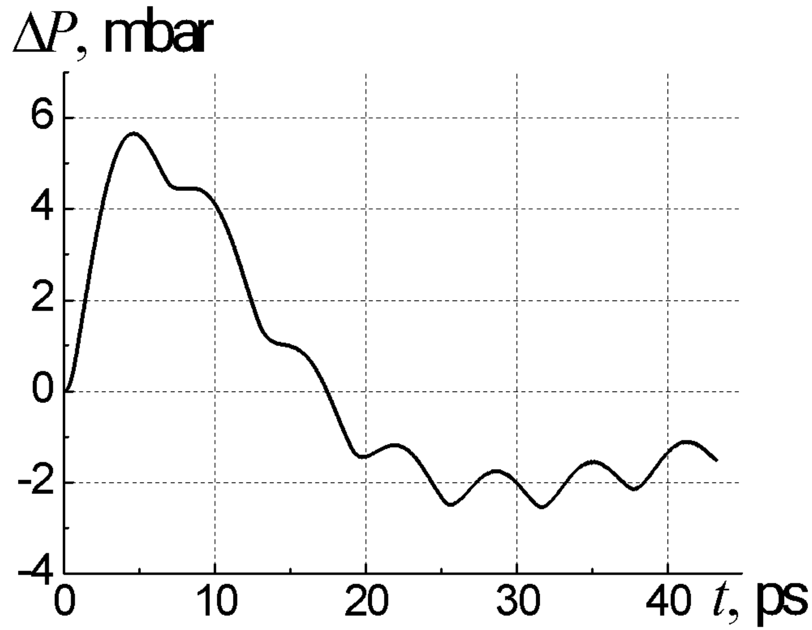
Oscillations of nanoparticle

Results and discussion

<u>Spherical geometry:</u> *gold nanoparticle in water*



$t_p=10^{-13}$s, $I_0=10^{10}$ W/cm^2

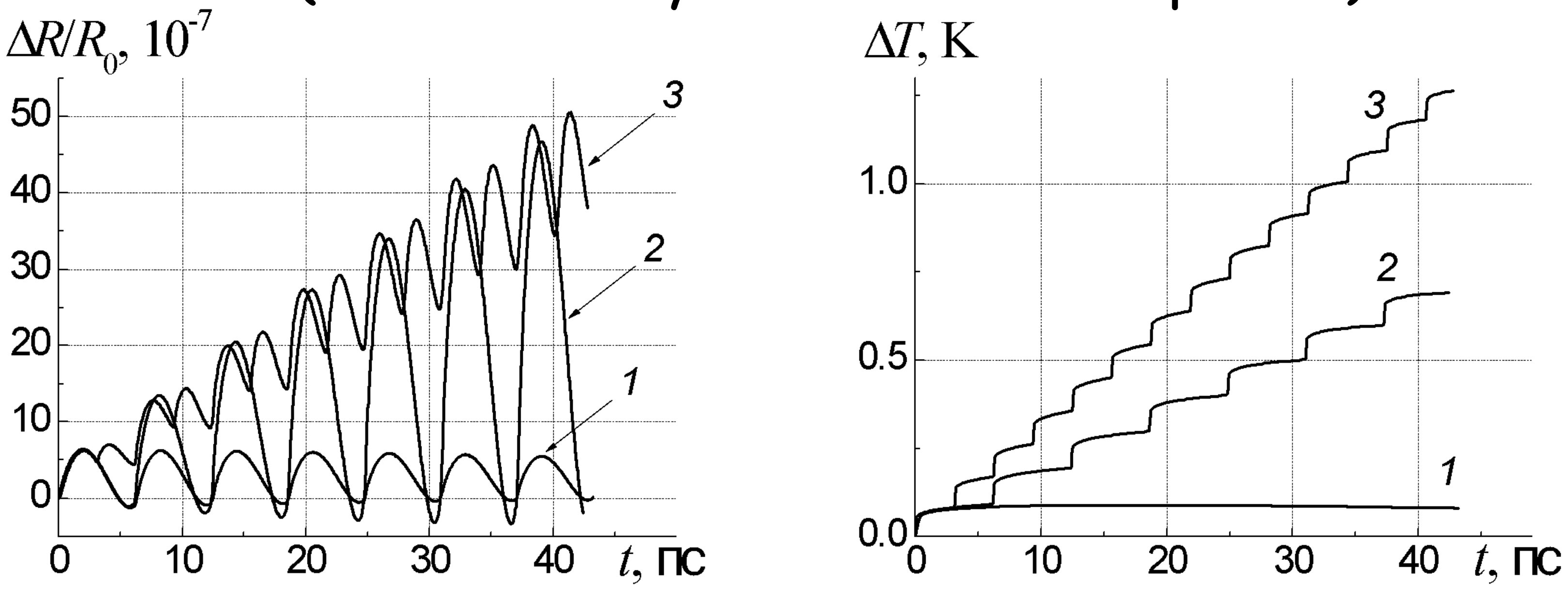


$t_p=10^{-11}$s, $I_0=10^{8}$ W/cm^2

Pressure oscillations outside the particle (r =1nm from surface).

Results and discussion

Gold nanoparticles in water (excitation by series of short pulses)

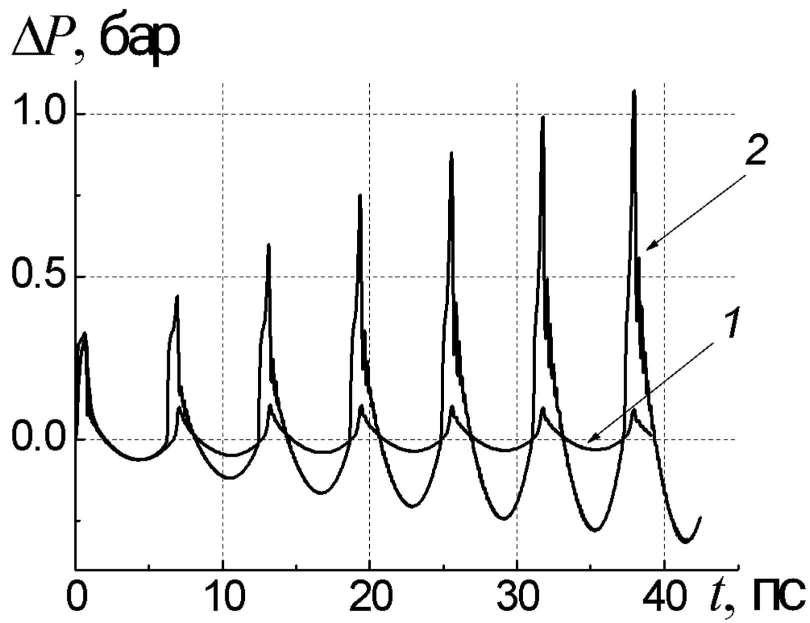


Oscillations of nanoparticle (*a*) and temperature in the centre of particle (*b*). *1* – single pulse; *2*, *3* – series of pulses. R_0=10 nm; $\tau_p=10^{-13}$ s; $I_0=10^{10}$ W/cm^2; ν = 160GHz (*2*), 320GHz (*3*).

Resonance enhancement of the oscillation amplitude

Results and discussion

Gold nanoparticles in water
(excitation by series of short pulses)



Pressure oscillations outside the particle (*r* =1nm from surface). 1 - single pulse; 2 – series of pulses, ν = 160GHz

Resonance enhancement of the oscillation amplitude

Conclusions

The theoretical model for thermomechanical action of ultrashort laser pulses on one-dimensional metallic nanostructures has been developed.
Heating of metals is described based on two-temperature model for an electronic gas and ionic lattice. Space-time dynamics of excitation and propagation of acoustic vibrations inside nanostructures and in a surrounding medium is investigated based on numerical solution of the equations for a continuous medium's motion in the Lagrange form.