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Investigation of interaction femtosecond laser pulses with skin and eyes mathematical model

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Abstract. We present a mathematical model of linear and nonlinear processes that takes place under the action of femtosecond laser radiation on the cutaneous covering. The study is carried out and the analytical solution of the set of equations describing the dynamics of the electron and atomic subsystems and investigated the processes of linear and nonlinear interaction of femtosecond laser pulses in the vitreous of the human eye, revealed the dependence of the pulse duration on the retina of the duration of the input pulse and found the value of the radiation power density, in which there is a self-focusing is obtained. The results of the work can be used to determine the maximum acceptable energy, generated by femtosecond laser systems, and to develop Russian laser safety standards for femtosecond laser systems.

Introduction
Femtosecond laser systems (FLSs) are widely used in science, technical applications and medical technologies [1, 2]. Despite the fast advancement of femtosecond technologies and their application in biology and medicine, currently, in the Russian Federation, there are no standards of safe energy levels of high-intensity femtosecond laser radiation. Note that the mechanism of interaction of intense femtosecond laser radiation with matter essentially differs from that for the pulses of longer duration, since the interaction time is smaller than the time, necessary to excite the phonon subsystem [3]. Besides, the high power density that arises when using the FLSs leads to various nonlinear processes, such as self-focusing, two- and three-photon absorption, multiphoton and impact ionization, and for the high energy density to the optical breakdown. [4]. This process is of particular importance in the case of femtosecond radiation incident on biological tissues, since the high-intensity femtosecond radiation may be essentially unsafe for skin, vision, and other human organs [5].

In the present work, we consider the linear and nonlinear interaction of femtosecond laser radiation with skin and eye and propose a mathematical model approximately describing particular interaction processes. In future, the model can be used to determine the maximal acceptable levels of FLS energy.

Interaction mechanism
1.1. Specific features of ultrashort-pulse lasers and the skin
The human skin is an optically turbid opaque medium (both the absorption and the scattering are present). At the same time, the skin is a heterogeneous structure containing the inclusions of different type and dimension (blood vessels, hair follicles, etc.), which essentially makes it difficult in the understanding of the processes that occur under the action of laser radiations on the cutaneous covering. The main constituents of the skin are water (70%) and proteins (27%), and the main structure protein is collagen (nearly 70% of dry skin weight). The water molecules can be divided into two groups, the free ones and the ones included in protein compounds (bound state, e.g., the three-fold
screw group of collagen binds nearly 500 water molecules [6]). Thus, in the first approximation the skin may be considered as water with protein inclusions close to dielectric materials in their electrodynamic properties.

Figure 1. Model of human skin.

The mean optical (λ=800 nm) and thermal physical parameters used in the skin model for calculating was taken from [7]. For estimation, we have chosen the wavelength 800 nm typical for the most commonly used titanium-sapphire FLSs. The pulse duration in such systems can vary from 25 to 550 fs. The irradiation with ultrashort laser pulses leads to damages that cannot be explained by the thermal melting mechanism [8] and are due to the excitation of valence electrons by the laser pulses [9, 10]. The water molecules serve as the transmitting element that absorb the laser pulse energy and excite the vibrational (phonon) modes of collagen with the relaxation time of the order of 3 ps [11, 12].

1.2. Mathematical model

In the calculations, we utilized the set of balance equations that describe the dynamics of electron-atom subsystem. In this model, the atoms interact via the semi empirical potentials and the electron degrees of freedom are not taken into account explicitly. The laser radiation generates non-equilibrium charge carriers described by the integral concentration [13]. In this case one can ignore the processes of Auger recombination and impact ionization, since for the chosen parameters of radiation their semi empirical contribution is negligibly small.

E.B. Yakovlev et al. [11] proposed the idea of determining the dependence between the potentials of the atoms and the state of the electronic sub-system, thus making it possible to simulate the effects of heat transfer under the action of femtosecond pulses on dielectric materials. The differential Bouguer-Lambert law determines the distribution of the laser radiation intensity J (z, t) inside a solid. The system of heat transfer equation that describe the dynamics of electron and atom subsystems in the one-dimensional approximation has the form:

\[
\frac{\partial T_e}{\partial t} = \alpha_e \frac{\partial^2 T_e}{\partial z^2} - \frac{1}{c_e^e \tau_{ep}} (T_e - T_0) + \frac{\alpha_e \hbar \nu}{c_e} J(t, z) \tag{1.1}
\]

\[
\frac{\partial T_a}{\partial t} = \alpha_a \frac{\partial^2 T_a}{\partial z^2} + \frac{1}{c_a \tau_{ep}} (T_e - T_a) \tag{1.2}
\]

where \( J(t, z) \) is the intensity distribution in the solid, \( C_e = \frac{\pi^2 k_B^2 N_e}{2 E_F} \) is the heat capacity of the electron gas, \( C_a \) is the heat capacity of atoms, \( \tau_{ep} \) is the time of electron-phonon relaxation, \( T_e \) is the temperature of electrons, \( T_a \) is the temperature of atoms, \( \alpha_e \) and \( \alpha_a \) is the thermal diffusivity of electrons and ions; \( E_F \) is the Fermi energy; \( K_B \) is the Boltzmann constant.

For modelling the impact of the femtosecond laser radiation on the skin we used the following boundary conditions:

\[
T_e \big|_{t=0} = T_0 \big|_{t=0} = T_0 \tag{2.1}
\]

\[
\frac{\partial T_e}{\partial z} \big|_{z=0} = \frac{\partial T_e}{\partial z} \big|_{z=L} = \frac{\partial T_a}{\partial z} \big|_{z=0} = \frac{\partial T_a}{\partial z} \big|_{z=L} = 0 \tag{2.2}
\]
The mechanism of effects on eyes

3.1 Features of the effects of radiation on the eye

Eye - is a complex self-regulating optical system, which is the scope of an average of about 24 mm in diameter (Figure 2). [14].

![Figure 2](image)

**Figure 2.** Schematic representation of the eye. In the upper part of the figure shows the refractive indices in the lower part - and the linear dimensions of the optical path-sky in mm [14].

Vitreous humor is mainly composed of water (99%), the balance being acetylcholine, protein, glucose, thiamine, pyridoxine, ascorbic acid, and proteolytic enzymes, little effect on the non-linearity of the medium. Thus, the major contribution to make the optical properties of water molecules.

On the optical path of the dispersion experiences femtosecond pulse broadening, which can be described by the formula [15]:

\[ n(\omega) = N_0 + a\omega^2 - b\omega^{-2} \]

where \( N_0, a, b \) - the dispersion characteristics of the medium.

The main danger for retina if laser radiation is heat exposure, which can lead to thermal and photochemical damage. However, when using pulsed radiation, femtosecond excited by electron subsystem that transfers the energy of the atomic subsystem, increases the time to reach a maximum temperature of [16]. At the moment, considering several theoretical models of optical damage mechanisms and biological objects, which are divided into mechanisms, associated with absorption, which include thermal explosion, and the internal mechanism - impact ionization and photoionization.

At 800 nm contribution to damage modify the main impact- and photoionization in the range of durations of 7 to 300 fs [17]. Photoionization is the dominant mechanism in a pulse length of less than 50 fs, and impact ionization becomes predominant in a pulse length of 50 fs more. [18]

1.2 Mathematical methods of calculation

The dynamics of a two-dimensional spectral density of g TE-polarized radiation in a homogeneous isotropic dielectric medium with a fast-response cubic nonlinearity can be described by the equation [19]:

\[ \frac{\partial^2 g}{\partial z^2} + (k(\omega) - k_x^2) g = \]

\[ -\frac{\omega^2 \varepsilon_{nl}}{c^2} \left( \frac{1}{2\pi^2} \right) \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} g(\omega - \omega', k_x - k_x', z) g(\omega' - \omega'', k_x' - k_x'', z) \]

\[ \times g(\omega'', k_x'', z) d\omega d\omega' d\omega'' d\omega''' d\omega''' d\omega''' \]

where

\[ g(\omega, k_x, z) = \int_{-\infty}^{\infty} E(t, x, z) e^{-i(\omega t + k_x x)} dt dx \]
w and \( k_x \) - temporal and spatial frequency of the radiation, \( k(\omega) \) - wave number, \( n(\omega) \) - the frequency dependence of the refractive index of the medium, \( \varepsilon_{nl} \) - coefficient of its nonlinear dielectric constant, \( c \) - speed of light in vacuum, \( t \) - time, \( x, z \) - Cartesian spatial coordinates, \( E(t, x, z) \) - the electric field radiation polarized perpendicular to the \( x_z \) plane.

The spectral density of the radiation entering the medium (at \( z = 0 \)) was set in the form:

\[
g(\omega, k_x, 0) = i g_0 e^{-\frac{\Delta x^2 k_x^2}{\omega_0}} \left( e^{\frac{\Delta t^2 (\omega - \omega_0)^2}{\omega}} - e^{-\frac{\Delta t^2 (\omega - \omega_0)^2}{\omega}} \right)
\]

where \( g_0 = \frac{\pi \Delta t \Delta x}{4} \sqrt{\frac{8\pi}{3N_0}} I_0 \) - maximum spectral density, \( \omega_0 \) - centre frequency, \( \Delta x \) - the transverse momentum of the size of the inlet to the environment, \( \Delta t \) - its initial duration, \( I_0 \) - radiation intensity.

Another boundary condition, which determines the direction of wave propagation, was reviewed in the linearized form:

\[
\frac{\partial g}{\partial z}_{z=0} = -i g(\omega, k_x, 0) \sqrt{k(\omega)^2 - k_x^2}
\]

To solve, equation (1) has used numerical scheme Crank-Nicholson adaptive step axis \( Z \). Convolution in the right-hand side of equation (1) is calculated using the fast Fourier transform algorithm. The calculation has been implemented in Fortran using OpenMP parallelization tools.

**Results**

4.1 For skin

By means of Monte Carlo numerical simulation of propagation of radiation through the skin tissues, we obtained the intensity distributions over the tissue depth. The calculation approximated the solution of the radiation transfer equation by modelling all possible photon trajectories passing through the skin tissue model. The steady-state form of the radiation transfer equation in a homogeneous medium can be written as the integral equation [20, 21]:

\[
L(r, s) = \int_0^\infty \exp(-\mu_{tr}R) \mu_s \int_{R-0}^{4\pi} \int_{R-0}^{4\pi} L(r' - Rs, s') d\Omega' dR
\]

where \( L \) is the luminance at the point \( r \) in the direction \( s \), considered for both the light source and for the radiation scattered towards the direction \( s \); \( R \) is the path length, \( Q \) is the light emitted in the direction \( s \) by the source at the point \( r - Rs \). The parameter \( \exp(\mu_{tr}R) \) determines the radiation transfer from the point \( r - Rs \) to the point \( r \). Thus, the first term in the equation characterises the light scattered at the point \( r - Rs \), from any direction \( s' \) to the direction \( s \), reaching the point \( r \), and the second term describes the light emitted from the point \( r - Rs \) in the direction \( s \).
Figure 3. The intensity of the radiation on the depth of penetration (at $\lambda = 800$ nm).

From fig. 3 investigation of interaction femtosecond laser pulses with skin and eyes mathematical model can see that at the depth of 0.3 mm the radiation intensity is below 30% of the initial level. It is known that the probability of multiphoton processes is directly proportional to the second, the third and higher powers of the laser intensity. Thus, the main nonlinear processes will take place in the upper skin layer, the epidermis.

The dynamics of the electron system can be described by the energy distribution. The state of the electron subsystem immediately after the impact, part of electrons transfers their energy to the atom subsystem as a result of relaxation more than 3 ps, when most part of the electrons has transferred their energy to the atom subsystem, the whole system tends to thermal equilibrium (fig. 4).

Figure 4. Thermodynamics of laser pulse, the dynamics of the electron gas temperature $T_e$, the dynamics of the crystal lattice temperature $T_a$.

The absorption of light quanta by no equilibrium electrons of the dielectric maximizes their kinetic energy. This leads to the increase of electron temperature during the light pulse, whereas the lattice remains practically cold. Therefore, one can group the process of the action of the femtosecond laser
radiation on the skin into three stages. At the first stage during the femtosecond pulse the multiphoton excitation of water molecules occurs. The energy of ionisation in this process amounts to 6.5 eV, so that to ionise one water molecule nearly 5 photons (800 nm) are needed, which is a cause for the reduction of the quantum efficiency ($\eta \leq 20\%$). Simultaneously the process of impact ionisation takes place. As a result, before the end of the laser pulse action $N_{max} \approx \eta \cdot E/\hbar \omega$ (E being the pulse energy) electrons will be excited to the upper ionised states of the water molecules with the energy above $U_i = 6.5$ eV. The second stage occurs after the action of the femtosecond pulse and lasts until the complete transfer of the energy from the electrons to the phonon subsystem. The electron gas is cooled and the collagen molecules are heated (tens of picoseconds). The third stage is the dissipation of heat over the bulk sample (a few microseconds).

We presented a mathematical model of the propagation of femtosecond radiation through the cutaneous covering. Using the Mote Carlo numerical simulation, we determined the dependence of the radiation intensity up-on the penetration depth. By the help of the analytical solution of the system of equations describing the energy balance between the electron subsystem and the atomic one, we considered the mechanism of the effect of femtosecond radiation on the skin and estimated the temporal processes that occur in the course of the femtosecond radiation acting on the skin.

4.2 For eye
The work shows that at wavelengths that are in the area of transparency of the eye media pulse, duration in contact with the retina cannot be less than 100 fs. Thus, the main mechanism of damage to the retina using FLS in this wavelength range will photo ionize.

Calculations show self-focusing in the vitreous occurs when power exceeds $10^{12}$ W/cm$^2$. If this power was recorded a significant increase in amplitude of the field on the retina. this near power density retina occurs when input power density of the radiation of about $10^6$ W / cm$^2$.

![Figure 5](image_url)

**Figure 5.** The graph of the spatial distribution of radiation intensity in the area of the retina to the initial duration of 10 fs (input into the eye) with an average wavelength of 800 nm.

Increasing the intensity when the input power density of the radiation $10^{12}$ W/cm$^2$ of 3%, and at a power density of radiation $5 \times 10^{12}$ W/cm$^2$ - about 15% of the input power. Note that the process of self-focusing is snowballing, so at higher power, the beam collapse does not give numerical simulation.

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