Mathematical simulation of kinetic processes in moving irradiated by neutrons gas medium containing uranium nanoparticles

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Abstract. The theoretical model and program complex for mathematical simulation of processes of transformation the nuclear energy into optical radiation energy was developed. The model includes the equations of gas dynamics, as well as the equations describing the kinetic processes in the non-equilibrium plasma excited by uranium fission fragments.
The kinetic processes in the moving irradiated by neutrons argon-xenon gas medium containing uranium nanoparticles was investigated.
The space-time evolution of this medium in nonuniform changing over time neutron field was studied. The space-time evolution of the gas parameters (temperature, density, velocity, pressure), as well as the distribution of the concentration of uranium nanoparticles under different initial velocities of the gas and the size of the nanoparticles was calculated.
The amplifying properties of a laser-active space-nonuniform nuclear-excited moving argon–xenon medium, containing uranium nanoparticles and irradiated by neutrons, was studied.

1. Introduction

There has been 40 years since it was proposed to use finely divided uranium-containing particles dispersed in an active gas medium to convert nuclear energy to optical radiation energy [1].

As compared to traditional techniques for heterogeneous nuclear pumping of active gas media, the use of finely divided uranium-containing particles may lead to the share of energy carried out by fission fragments from condensed phase into the gas medium to increase tenfold and more. This creates opportunities for improving the efficiency of nuclear energy conversion to optical radiation energy.

Dispersal and absorption of laser radiation (LR) by an active medium with a content of finely divided uranium-containing particles is a major factor that hampers the generation of laser radiation in this medium.

It has been proposed recently to use laser-active gas media irradiated by neutrons and containing nanoclusters of uranium compounds [2].

In the beginning of computational and theoretical studies, the number of models and complexes of programs for mathematical modeling of kinetic processes in argon-xenon plasma irradiated by neutrons and containing uranium nanoparticles were designed [2-6]. Using developed models and programs it was demonstrated that it was possible to amplify laser radiation in a nuclear-excited argon–xenon dusty gas plasma [2, 3, 6].

It was further shown by mathematical modeling methods that during generation of laser radiation (LR) in an argon–xenon gas medium irradiated by neutrons and containing uranium nanoparticles the conversion of the uranium fission fragment kinetic energy to LR energy was an order of magnitude as efficient as the conversion of this energy during heterogeneous pumping [7-9].

This makes it possible to expect that a method and devices will be developed with a high efficiency of direct conversion of the fission fragment kinetic energy to the energy of coherent optical radiation.

In [7-9] however, only an immovable homogeneous dusty medium was considered. To prevent uranium nanoparticles from depositing in gas, it appears to be reasonable to blow down this medium. Apart from that, a dusty medium may start to move in the process of irradiation when the heating of gas by fission fragments is non-uniform.

Mathematical modeling of kinetic processes in a laser-active element (LAEL) in a moving argon–xenon gas medium containing uranium nanoparticles, during steady motion was developed in [10-12].

This paper deals with mathematical modeling of kinetic processes in argon-xenon plasma irradiated by neutrons and containing uranium nanoparticles, during unsteady motion of the medium, caused by pumping of this medium through LAEL, and heating of it by neutron-induced spatiotemporal inhomogeneous field of uranium fission fragments as well.

The purpose of the study is to determine the effects of the active medium movement and the spatial non-uniformity on the LR amplification process in a LAEL.

2. The main equations of the model

Let's investigate spatiotemporal evolution of moving into LAEL argon-xenon plasma containing uranium nanoparticles. LAEL is a cylindrical tube of radius R and length Z.

Due to high penetrating ability of neutrons at near to the perpendicular direction of incidence of neutron radiation on LAEL axis can confine ourselves to the study of axially symmetric motion of the gas in it.

We use to describe the spatiotemporal evolution of gas continuity equation environment, the Navier-Stokes equations, the energy balance equation, as well as the transfer of nanoparticles based on convection and diffusion, which in a cylindrical coordinate system are:

$$\frac{\partial \rho}{\partial t}+div\left(\rho \vec{V}\right)=0, \tag{1}$$

$$\frac{\partial \rho u}{\partial t}+div\left(\rho u\vec{V}\right)=-\frac{\partial p_t}{\partial z}+S_u, \tag{2}$$

$$\frac{\partial \rho v}{\partial t}+div\left(\rho v\vec{V}\right)=-\frac{\partial p_t}{\partial r}+S_v, \tag{3}$$

$$\rho c_p\frac{\partial T}{\partial t}+\rho c_p\vec{V}gradT=div\left(\lambda_t gradT\right)+\frac{dp_t}{dt}+Q, \tag{4}$$

where

$$S_u=-\frac{2}{3}\frac{\partial}{\partial z}\left(\mu div\vec{V}\right)+\frac{1}{r}\frac{\partial}{\partial r}\left[r\mu\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial z}\right)\right]+2\frac{\partial}{\partial z}\left(\mu\frac{\partial u}{\partial z}\right), \tag{5}$$

$$S_v=-\frac{2}{3}\frac{\partial}{\partial r}\left(\mu div\vec{V}\right)+\frac{\partial}{\partial z}\left[\mu\left(\frac{\partial u}{\partial r}+\frac{\partial v}{\partial z}\right)\right]+2\frac{\partial}{\partial r}\left(\mu\frac{\partial v}{\partial r}\right)+2\mu\frac{\partial}{\partial r}\left(\frac{v}{r}\right), \tag{6}$$

$$\frac{\partial N}{\partial t}=D_f\left(\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial}{\partial r}N+\frac{\partial^2}{\partial z^2}N\right)-\frac{1}{r}\frac{\partial}{\partial r}rj_r-\frac{\partial}{\partial z}j_z\,. \tag{7}$$

Here z, r – cylindrical (axial and radial) coordinate, ρ, c_p, T – density, specific heat at constant pressure and temperature; u, v – axial and radial components of velocity $\vec{V}$; p_t – gas pressure; μ – dynamic viscosity and λ_t – gas thermal conductivity; Q – the volumetric power density of fission fragments in the gas, for heating the heavy gas particles (atoms, ions), N – concentration of uranium nanoparticles, D_f – diffusion coefficient of uranium nanoparticles, $\vec{j}$ – the density of the dust particle flow equal to

$$\vec{j} = \vec{v}_p N , \tag{8}$$

containing $\vec{v}_p$ – the dust particle movement velocity, which may differ from the argon–xenon gas medium movement velocity.

Next we confine ourselves to spherical nanoparticles with radius r_p which is less than a few tens of nanometers, which in dense gas (~ 1 atm pressure) moving along with the gas. Then we can assume that $\vec{v}_p$ is the same as the velocity of the gas.

We shall determine the diffusion coefficient D_f using the approximation proposed in [13]:

$$D_f = \frac{k_B T\left(1+3{,}12\mathrm{Kn}\right)}{6\pi r_p \mu}, \tag{9}$$

where $\mathrm{k_B}$ – Boltzmann constant; Kn – Knudsen number.

3. The power density of fission fragments calculation in LAEL

In LAEL with gas containing nanoparticles of the energy from uranium fission fragments at the coordinates r, z can be defined as the divergence of the energy flux density transported by fission fragments, followed by integration over the volume of LAEL:

$$Q(r,z) = \sum_{i=1}^{n_f} \int_0^{2\pi} d\varphi \int_0^{z_m} dz_1 \int_0^{R} r_1 dr_1 \frac{S_0(r_1,z_1)}{\pi l^2} \left| \frac{\partial T_i(l')}{\partial l'} \right| \frac{\rho(r_1,z_1)}{\rho_0}, \tag{10}$$

containing z_m - the maximum of z, with which uranium fission fragments could reach destination point of calculations, n_f - the number of uranium fission fragments per fission act, $S_0(r_1,z_1)$ - the fission speed in unit volume at point with r_1, z_1, $T_i(l')$ - the energy of fission fragment i, which passed effective distance $l' = \int_0^l \frac{\rho}{\rho_0} dl$, $l = \sqrt{r^2 + r_1^2 - 2rr_1\cos\varphi + z^2}$ - real distance, which fission fragment passed in the gas, r_1 - the distance from the axis of LAEL to fission fragments' source, φ - the angle between directions from the axis of LAEL to the source of fission fragments source on a given point in the cross section, ρ_0 - the normal density of the gas for which the specified dependency $T_i(l)$.

Since the characteristic length in the longitudinal heterogeneity in LAEL, usually much larger than its radius, then, considering the subsonic gas motion may be presented in the form of two components

$$p_t = p_0 + p, \tag{11}$$

where p_0 – the average LAEL's cross-section pressure depends only on the coordinates z, p – component of the pressure, which depends both on the coordinates z, and r, and we can assume that

$$p_0 \gg |p|. \tag{12}$$

Neglecting in (4) p as compared to p_0 and integrating (4) over the cross section of LAEL from z_1 to z_2, taking into account (1) it can be obtained for p_0 the following equation

$$\frac{3V_0}{2}\frac{\partial p_0}{\partial t} = \int_{V_0} QdV - \int_{S_0} \lambda_t gradTd\vec{S} - \int_{z=z_1} udS - \int_{z=z_2} udS, \tag{13}$$

where V_0 - the volume by which the integration is, the S_0 - surface bounding this volume. The last two integrals in (13) are taken in cross-section of LAEL at a fixed z.

Taking into account (11), (12), and that the average pressure varies only along the coordinate z, Navier-Stokes equations can be rewritten

$$\frac{\partial \rho u}{\partial t} + div\left(\rho u\vec{V}\right) = -\frac{\partial p_0}{\partial z} - \frac{\partial p}{\partial z} + S_u, \tag{14}$$

$$\frac{\partial \rho v}{\partial t} + div\left(\rho v\vec{V}\right) = -\frac{\partial p}{\partial r} + S_v. \tag{15}$$

Boundary conditions

$$z=0,\ u=u_{\max}(1-r^2/R^2),\ v=0,\ T=T_{z0},\ \ p_t=p_0,\ N(z,R,t)=N_0(R); \tag{16}$$

$$r=0,\ \frac{\partial u}{\partial r}=0,\ v=0,\ \frac{\partial T}{\partial r}=0,\ \frac{\partial p_t}{\partial r}=0; \tag{17}$$

$$r=R,\ u=v=0,\ T=T_R(r,t),\ \frac{\partial p_t}{\partial r}=0,\ \ N(z,r,t)=0; \tag{18}$$

$$z=Z,\ \frac{\partial u}{\partial z}=\frac{\partial v}{\partial z}=0,\ \frac{\partial T}{\partial z}=0,\ \frac{\partial p_t}{\partial z}=0,\ \frac{\partial N(0,r,t)}{\partial z}=N_0 \tag{19}$$

To solve the system of equations (1) - (19) the method of finite differences was used. These equations were approximated using five-point finite-difference scheme. The solution method is described in detail in [14-16].

4. Results of spatiotemporal argon-xenon gas medium containing uranium nanoparticles evolution modeling

Figures 1–4 show typical results of the space-time evolution of the velocity distribution in the projection of LAEL its temperature axis, pressure and concentration of uranium nanoparticles. The distribution of the power in LAEL axis at different times are shown on figure 5.

Results of calculations are shown for the particles with a radius in $r_p = 5$ nm and $p = 0.5$atm initial gas pressure and the following values of the variables: $Z = 300$ cm, $R = 12$ cm, $u_{\max} = 2$ m/s, the maximum concentration of uranium particles on LAEL axis was assumed to be $N_0 = 10^{12}$ cm^{-3}. The dependence of the thermal neutron flux density J, causing fission of uranium nuclei, given as

$$J = J_0 \exp(1-(t/\tau_0)-((z-Z/2)/(Z/6))^2)(t/\tau_0), \tag{20}$$

where $\tau_0 = 150$ ms.

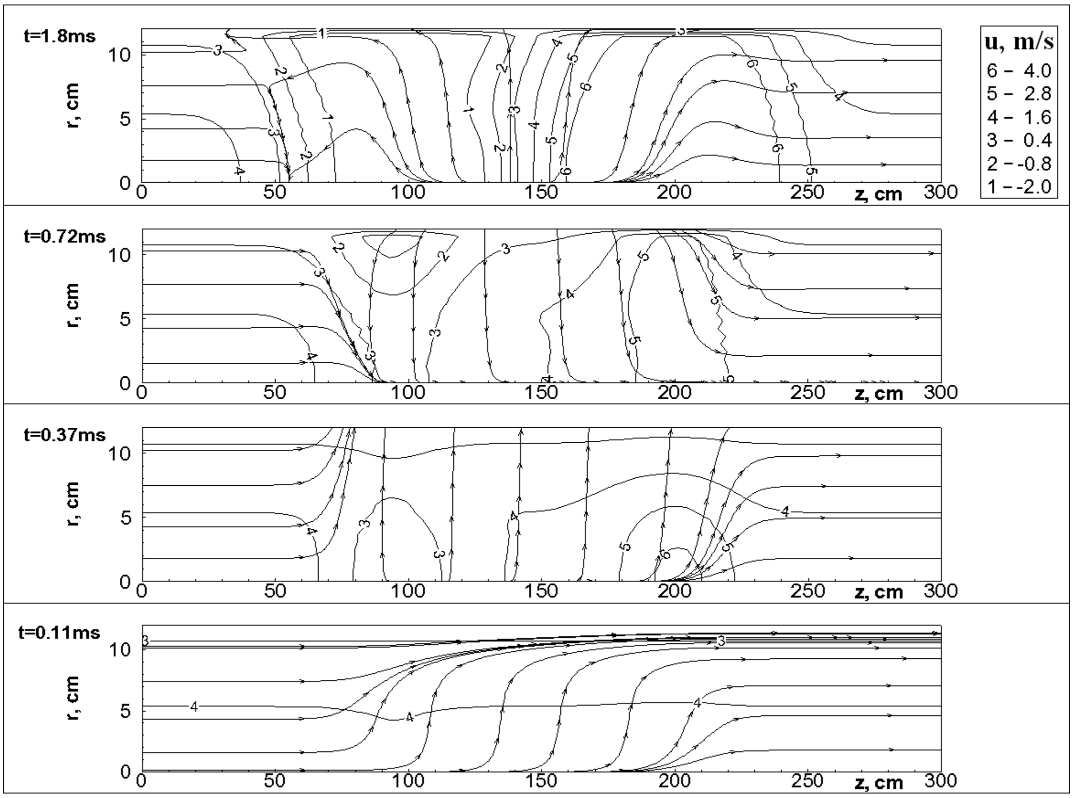

Figure 1. The distribution of the speed projection u to LAEL's axis at different times.

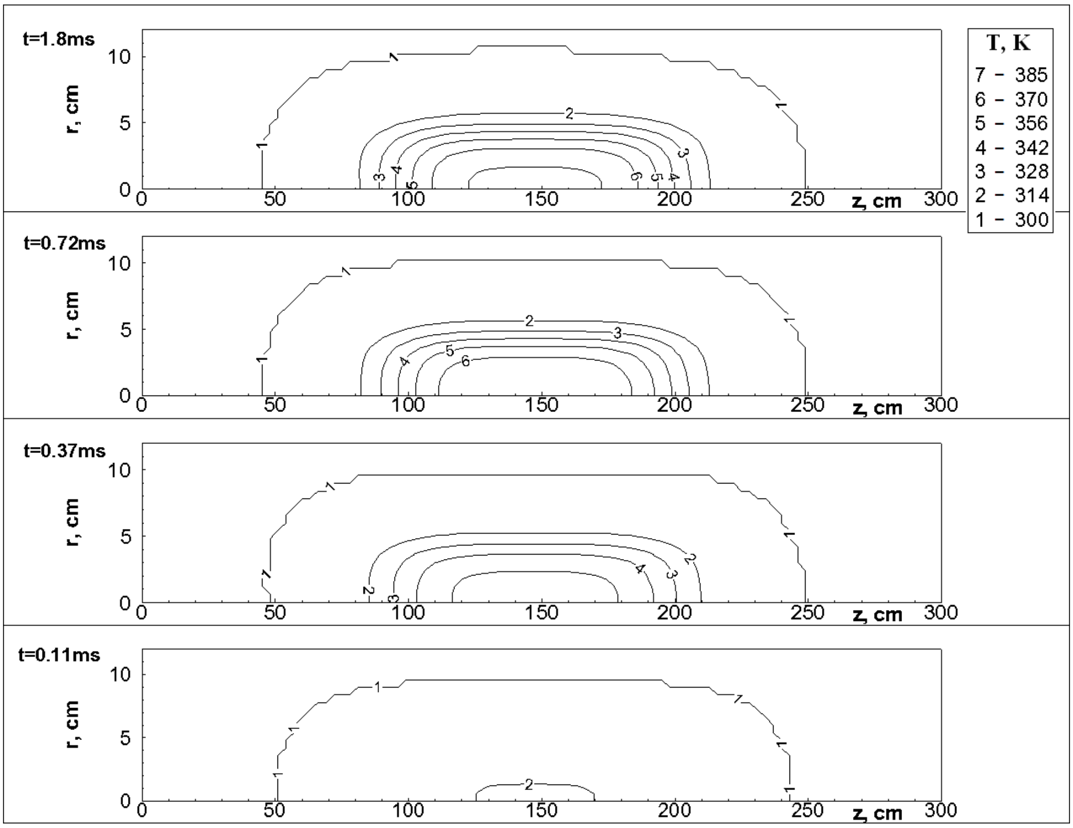

Figure 2. The distribution of the temperature in LAEL at different times.

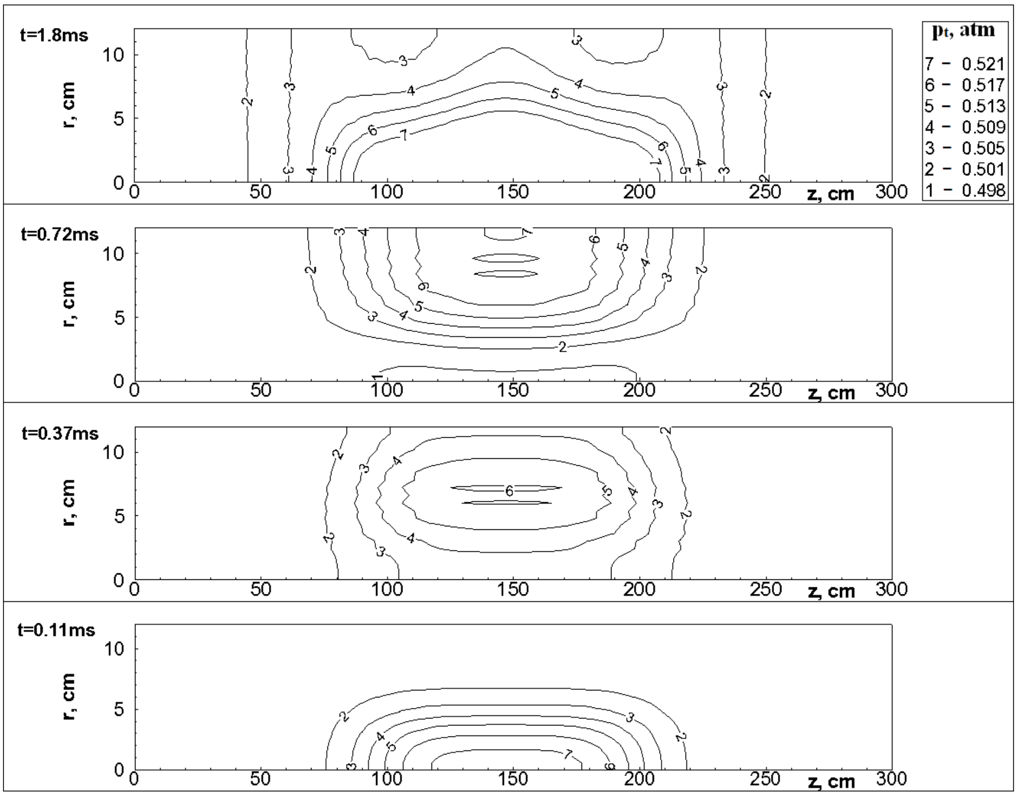

Figure 3. The distribution of the pressure in LAEL at different times.

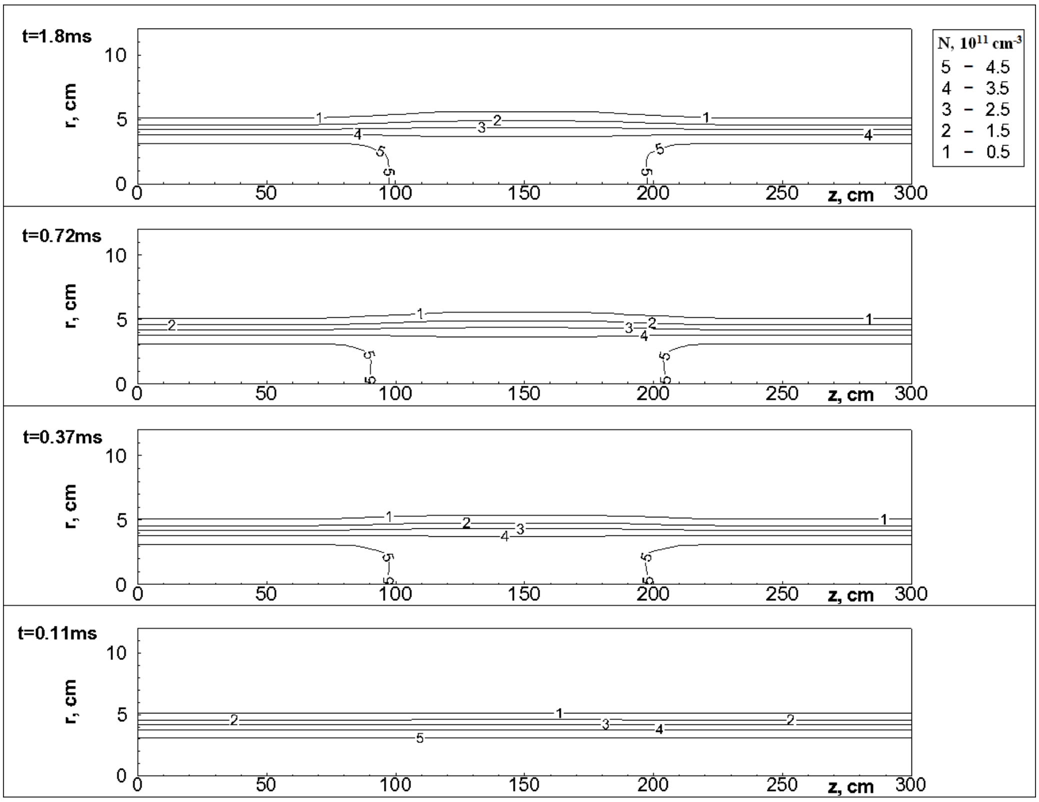

Figure 4. The distribution of the concentration of nanoparticles in LAEL at different times.

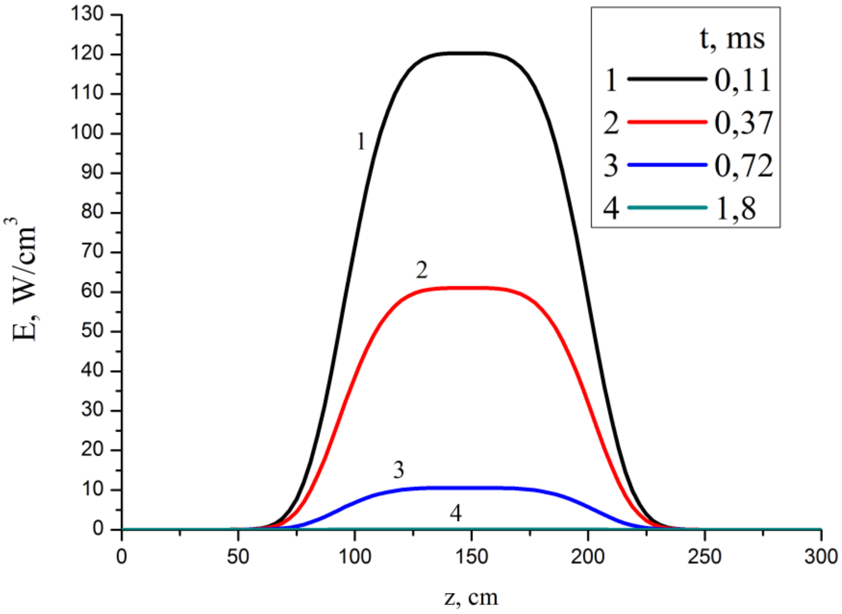

Figure 5. The distribution of the power in LAEL axis at different times.

5. A model of kinetic processes in a dusty argon–xenon laser-active medium excited by fission fragments

A model of kinetic processes in an argon–xenon laser-active medium with a monodispersed dusty component excited by fission fragments was developed in [2, 3]. This model was used in the present study to investigate the kinetic processes in the plasma created by neutron-induced uranium fission fragments.

The kinetic model of an argon–xenon medium with a monodispersed dusty component in the gas component took into account the atomic (Ar^+, Xe^+)and homonuclear molecular (Ar_2^+, Xe_2^+) ions of argon and xenon, the heteronuclear ion $ArXe^+$ and the molecule $ArXe$, argon and xenon molecules in excited states, as well as argon and xenon excimers (Figures 6, 7).

Levels 6s, eight 5d sublevels and six 6p sublevels were considered separately for the excited xenon atom, and the sublevels of the states and 7s were combined to form a single level Xe(p s) (Figure 6). All other xenon states were combined to form a single state designated Xe*.

The sequence of the major kinetic processes leading to the formation of an inverse population in the argon–xenon medium is as follows. While interacting with the argon–xenon medium, fission fragments lose energy, primarily for the formation of atomic ions and excited argon atoms. Further, the collision of atomic ions Ar^+ and excited argon atoms with argon and xenon atoms leads to the formation of both excited xenon atoms and the atomic xenon ions Xe^+, as well as of the molecular homonuclear ions $\mathrm{Ar}_2^+, \mathrm{Xe}_2^+$ and the heteronuclear ions.

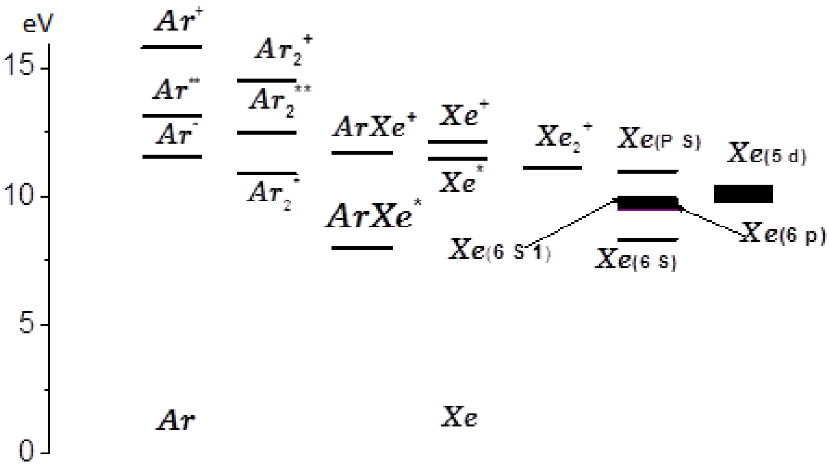

Figure 6. Energy diagram of states considered in the kinetic model.

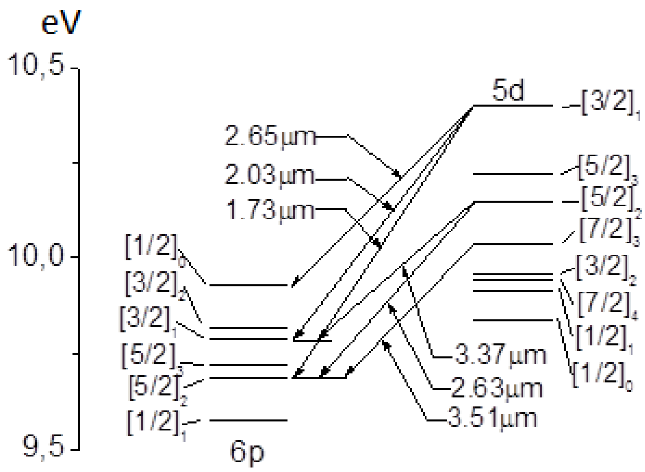

Figure 7. Energy diagram of the xenon atom states considered in the kinetic model at the transition between which it is possible to achieve the generation of laser radiation.

Check the upper excited states of xenon atoms (denoted as PS) procomes as a result of dissociative recombination of molecular ions $ArXe^{+}$, Xe_2^{+}. In the future as a result of collisions with argon atoms going population of the upper levels for the transitions with a wavelength of 1.73 micron, 2.03 micron and 2.65 micron.

The up and lower laser levels are populated through multiple channels - due to quenching of excitation in the collision ions with the plasma electrons and by radiation as a result of stimulated and spontaneous emission. These processes lead to the population of the lower laser levels, which are extinguished in collisions with argon atoms and electrons, settling with a low-lying excited states of xenon atoms. These processes lead to the population of the lower laser levels, which are extinguished in collisions with argon atoms and electrons, settling with a low-lying excited states of xenon atoms.

In the model with a monodisperse dust component of the processes of interaction of electrons and ions with the charged nanoparticles are described as follows "plasma chemical" reactions:

$$e + D \to D(-), \tag{21}$$

$$e + D(n-) \rightarrow D((n+1)-)\,, \tag{22}$$

$$I(+) + D(n-) \rightarrow D((n-1)-)\,, \tag{23}$$

$$I(+) + D \rightarrow D(+)\,. \tag{24}$$

Here we have introduced the notation e – electron, D, $D(+)$, $D(n-)$ – respectively, are electrically neutral, positively and negatively charged nanoparticles 5 nm in radius, n - charge of the nanoparticles in units of electron charge, $I(+)$ - any positively charged atomic or molecular ion of the gas mixture.

Altogether, 57 components were considered and 434 reactions in the argon–xenon medium were taken into account in the model.

6. LR linear amplification by medium coefficient calculation

An important characteristic of the laser-active medium is a gain of the linear laser light. Using the model kinetic processes in a xenon-argon plasma containing uranium nanoparticles may define unsaturated linear laser gain.

In mathematical modeling of the microscopic kinetics of the following circumstances may be used. In typical conditions, the nuclear pump power density of the energy input into the laser-active medium is changed slowly over time (the characteristic time changes $\tau \geq 10$ ms). Diffusion of plasma components can be neglected, because of the characteristic lifetime of most of the major components of argon-xenon medium diffusion length is much smaller than the characteristic spatial scales of energy irregularities. This allows the steady-state approximation of the local kinetics - that is, assume that the concentration of various components of the plasma at a given point are determined by the instantaneous values of the temperature of the heavy particles, gas pressure and power density energy deposition in the local approximation.

In operation, the values were calculated quasistationary linear gain laser radiation at a wavelength of 1.73 microns at a concentration of uranium in the range of nanoparticles $0.125 \cdot 10^{11}$ cm^{-3} to 10^{12} cm^{-3}, LAEL gas pressure in the range of 0.5 atm to 0.6 atm and the specific energy input power ranging from 23 W/cm^3 to 277 W/cm^3.

The table 1 shows typical results, whether linear IS gain calculation gaseous medium quasistationary values at a wavelength of 1.73 microns, depending on the concentration of uranium in the nanoparticulate active laser-xenon, argon-gas atmosphere at a specific energy input power of 230 W/cm^3at different gas pressures in LAEL.

The gain of the laser gas medium is designed to disregard the weakening of nanoparticles radiation. There's also shows the calculated data on the dependence coefficients attenuation β laser attenuation uranium nanoparticles (the particle radius - 5 nm) on their concentration for a wavelength of 1.73 microns [2,3,5,6] and the value of the total gain medium, calculated by formula:

$$k = \alpha - \beta\,. \tag{25}$$

To calculate the total gain medium LAEL containing uranium nanoparticles over the entire range of possible values, the method of linear interpolation based on the calculated parameters of the gain medium.

The changing of intensity I of the laser radiation propagating parallel to the cylinder axis, can be described by the following equation:

$$\frac{dI}{dz} = k\left(z, r, t\right) I \tag{26}$$

We define the LR intensity by gas medium containing uranium nanoparticles gain as follows:

$$K(z,r,t) = I / I_0, \quad (27)$$

where I_0 - the intensity of the radiation entering the laser active medium.

Then $K(z,r,t)$ can be written as:

$$K(z,r,t) = \exp(\int_0^z k(z_1,r,t)dz_1) . \quad (28)$$

Table 1. Linear gains α of the gaseous medium, the attenuation β of the radiation to depending on the concentration of nanoparticles N and gas pressure and the full gain of the medium k at a temperature T = 300 K, and the specific energy input power of 230 W/cm^3.

P, atm	N, 10^{10}cm^{-3}	α, 10^{-2}cm^{-1}	β, 10^{-3}cm^{-1}	k, 10^{-2}cm^{-1}
0.5	100	4.4	2.1	4.2
	50	4.5	1.09	4.4
	25	4.5	0.5	4.5
	12.5	4.6	0.2	4.5
	10	4.6	0.2	4.6
	5	4.6	0.109	4.6
	2.5	4.6	0.05	4.6
	1.25	4.6	0.02	4.6
0.6	100	4.3	2.1	4.1
	50	4.4	1.09	4.3
	25	4.4	0.5	4.4
	12.5	4.5	0.2	4.4
	10	4.5	0.2	4.5
	5	4.5	0.109	4.5
	2.5	4.5	0.05	4.5
	1.25	4.5	0.02	4.5

In the quasi-stationary approximation the local kinetics using data calculations spatio-temporal evolution of environmental parameters (temperature distribution, pressure, concentration of uranium nanoparticles, specific power input energy of fission fragments) and neglecting the refraction of the laser, we can estimate the gain of the laser intensity considered laser-active medium.

Figure 8 shows the results of radial dependence of the intensity $K(z,r,t)$ LR gain at different times from the outlet LAEL.

Conclusion

A two-dimensional non-uniform axial-symmetric model was developed to describe the space-temporal evolution of the concentration of uranium nanoparticles in LAEL. . Also the finite difference method for numerical solution of the model equations was designed.

The mathematical simulation of kinetic processes during direct conversion of the kinetic energy of the uranium fission fragments into the laser energy in the dust LAEL containing uranium nanoparticles was carried out.

The motion of the dusty nuclear-exited plasma induced by forced blowing of gas medium in LAEL and by the nonuniform energy release in the fission fragments' medium irradiated by unsteady space-nonuniform neutron field was investigated.

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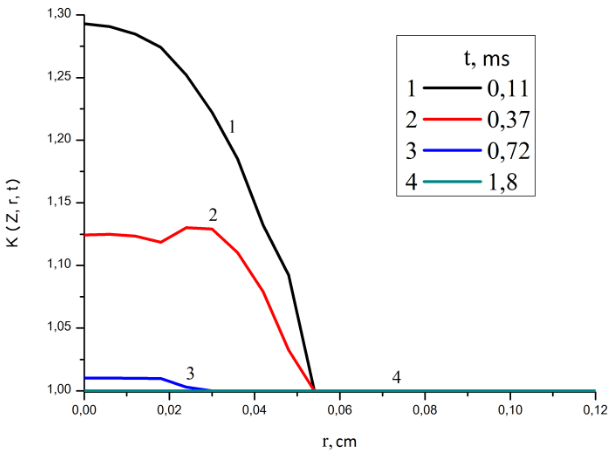

Figure 8. Radial dependence of the LR intensity amplification coefficient at different times.From these results of calculations of the gain of laser intensity, it follows that the medium length of 1 m provides a significant amplification of laser radiation in a single pass.

The space-time evolution of the gas parameters (temperature, density, velocity, pressure), as well as the distribution of the concentration of uranium nanoparticles under different initial velocities of the gas and the size of the nanoparticles was calculated.

Using the results of these calculations in the local microscopic plasma chemical kinetics quasi-stationary approximation it possible to determine the most important characteristics of the active medium - quasi-stationary value of the linear gain of LR at a wavelength of 1,73 microns.

The amplifying properties of a laser-active space-nonuniform nuclear-excited moving argon–xenon medium, containing uranium nanoparticles and irradiated by neutrons allow you to use such medium not only in nuclear pumped lasers but also in optical quantum amplifiers with nuclear pumping.

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