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ДИНАМИКА ТЕРМОФИЗИЧЕСКИХ ПАРАМЕТРОВ АБЛЯЦИОННЫХ ФАКЕЛОВ СЕРЕБРА ПРИ АТМОСФЕРНОМ ДАВЛЕНИИ

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Описан подход к моделированию термодинамических параметров пара в абляционном факеле серебра, распространяющемся при атмосферном давлении. Предлагаемая полуэмпирическая модель основана на модификации модели Анисимова – Лукьянчука с учетом теории динамической конденсации Зельдовича – Райзера. Процесс динамической конденсации сферических (или полусферических) абляционных факелов можно графически представить как прохождение в расширяющемся пароплазменном облаке от периферии к центру трех пространственных концентрических сферических волн. Это волна «насыщения» (соответствующая моменту пересечения пуассоновской адиабаты с адиабатой насыщения на фазовой диаграмме состояний пара), волна «впрыскивания» зародышей будущих капель (момент наибольшего переохлаждения пара в факеле) и волна «закалки» (стабилизация степени конденсации пара в факеле). Благодаря модификации ряда оснований модели Анисимова – Лукьянчука удалось предложить адекватное описание термодинамических процессов, протекающих при нормальном атмосферном давлении.

Ключевые слова: абляционный факел; теория Зельдовича – Райзера; динамическая конденсация; наночастицы металлов.

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DYNAMICS OF THERMOPHYSICAL PARAMETERS OF SILVER ABLATION JETS AT ATMOSPHERIC PRESSURE

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The paper demonstrates an approach to modeling the thermophysical parameters of vapor in an ablative silver jet propagating at atmospheric pressure. The proposed semi-empirical model is based on the modification of the Anisimov – Luk'yanchuk model taking into account the Zeldovich – Raiser dynamic condensation theory. Such process of dynamic condensation of spherical (or semi-spherical) ablative jets can also be graphically represented as passing in the expanding vapor-plasma cloud of the three spatial concentric spherical waves from the periphery to the center of cloud. There are «saturation» wave (corresponding to the moment of crossing the Poisson adiabate with saturation adiabate at the phase diagram of vapor), wave of nuclear «etching» (the moment of greatest supercooling of vapor in the jet) and the «quenching» wave (stabilization of the condensation degree of the vapor in the jet). Due to the revision of a number of basements of the Anisimov – Luk'yanchuk model, it was possible to offer an adequate description of thermodynamic processes occurring at normal atmospheric gas pressure.

Keywords: ablative jet; the theory of Zeldovich – Raiser; dynamic condensation; nanoparticles of metals.

Introduction

The modes of laser ablation of metals have attracted the attention of researchers since the creation of the first laser sources of optical radiation in the middle of the last century. The description of the laser ablation jet expansion is associated with many fundamental difficulties. We can observe the complex phenomenon of the interaction of high-power pulsed laser radiation with a metal lattice, which leads to inhomogeneity and unsteadiness of resulting plasma jet. Experimental investigation of the laser ablation of metals is further complicated by the interaction of the jet with incident laser radiation and the significant influence of surrounding gases [1; 2]. At the same time, the modes of high-power nanosecond laser pulses are of considerable interest for research, since the duration of the leading edge of such pulses becomes comparable with the characteristic time scale of relaxation processes in a metal lattice, which allows us to develop extreme methods of metal processing [3].

The «hydrodynamic» model or the «explosive ablation» model can be used to describe such ablation processes [4]. The «hydrodynamic» model name follows the assumption that the initial dynamics of a plasma jet can be described by a complete system of hydrodynamic equations. It is assumed that at the initial stages of development of the ablative jet, its vapor exhibits behavior characteristic of a dense incompressible liquid. When modeling such processes, the complete system of hydrodynamic equations underlying the «hydrodynamic» model should be supplemented with the equation of state of the target substance and data on its heat capacity, thermal conductivity and electrical conductivity in a wide area of the phase diagram of states (including the critical point and the two-phase region). A consistent theory that reliably models such phenomena is currently not developed, and the available experimental facts are very limited [4]. This significantly limits the wide application of the «hydrodynamic» model to describe real ablation processes.

Nevertheless, S. I. Anisimov and B. S. Luk'yanchuk proposed a comparatively complete model for describing the processes occurring in such vapor jets after finishing of their formation (i. e., when their interaction with incident radiation stops). The model [4–8] is based on the application of the adiabatic expansion approximation of an axisymmetric or spherically symmetric vapor-plasma cloud with parabolic or rectangular initial internal temperature and density profiles into a vacuum, taking into account the processes of dynamic condensation according to the Zeldovich – Raiser theory [9]. Comparison of simulation results for Si, Ge and C jets (with initial conditions corresponding to laser ablation of these materials by intense nanosecond pulses) with experimental data [10] showed their good agreement even in the absence of fitting parameters.

In earlier papers [11; 12] it was made the adaptation of the main aspects of the Anisimov – Luk'yanchuk model to describe the processes occurring in ablative lead jets at atmospheric pressure. However, the problems of studying ablative jets of precious metals are of much greater practical interest, since they can serve as a source of the nanoscale phase of these metals, suitable for the formation of promising nanostructured materials. This article describes the dynamics of thermophysical parameters of ablative silver jets formed under conditions identical to nanosecond laser action and propagating at atmospheric pressure.

Model of propagation of silver ablation jet after exposure of a nanosecond laser pulse

In the Anisimov – Luk'yanchuk model, the following spherically symmetric model is proposed to describe the dynamics of expansion of an ablative jet into a vacuum [4]:

$$\Psi(t)=\left(\frac{R(t)}{R_0}\right)^2=1+2\frac{u_0}{R_0}t+\left[\left(\frac{u_0}{R_0}\right)^2+\frac{16E}{3MR_0^2}\right]t^2, \tag{1}$$

where $\Psi(t)$ – dimensionless function, describing the magnitude distribution of the leading edge of a spherical jet; $R(t)$ – dependence of the spherical jet radius on time; R_0 – initial radius of the jet; u_0 – initial velocity of jet propagation; E – initial internal energy of the jet vapor; M – mass of jet vapor.

At work [13], processes accompanying the laser ablation of metal (Pb, Zn, Cu, Ni, Ag, Au, Pt) targets at atmospheric pressure were studied. Parameters of laser pulses are: duration 20 ns, energy in pulse 200–300 mJ, power density 10^8–10^9 W/cm^2. Using experimentally determined data [13]: $u_0 = 7.1$ km/s; the average mass removed per pulse, $M = 0{,}15 \cdot 10^{-8}$ kg. Value $E = 1.5$ mJ is calculated using data [14] on the characteristic value of ablative loading of metals (the share of the energy of the affected radiation converted into the kinetic energy of the jet). At fig. 1, the solid curve corresponds to the substitution of the set initial data for silver ablative jet in (1). However, as it was noted at [12], this approximation gives a highly inflated jet size for lead ablative jet in comparison with experimental data [13] (which is not surprising, given the orientation of this approximation to the expansion of jet in a vacuum).

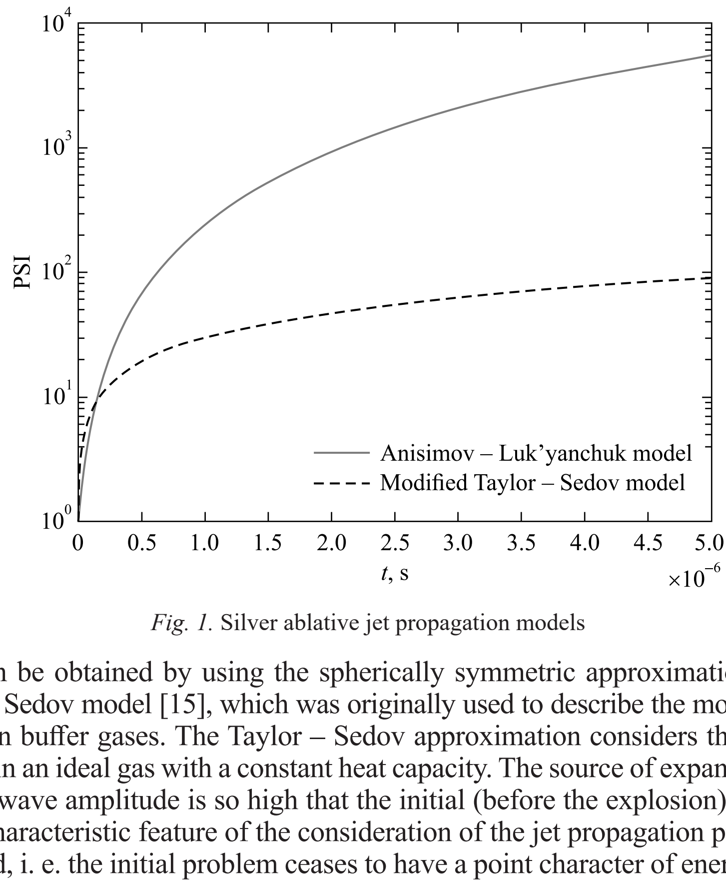

Fig. 1. Silver ablative jet propagation models

The better effect can be obtained by using the spherically symmetric approximation based on a modification [12] of the Taylor – Sedov model [15], which was originally used to describe the movement of the front of an explosive shock wave in buffer gases. The Taylor – Sedov approximation considers the case of propagation of a spherical shock wave in an ideal gas with a constant heat capacity. The source of expansion is a short-term point energy release, and the wave amplitude is so high that the initial (before the explosion) parameters of the buffer gas can be ignored. A characteristic feature of the consideration of the jet propagation process is the existence of an initial spherical cloud, i. e. the initial problem ceases to have a point character of energy input into the system.

This requires a corresponding transformation of the Taylor – Sedov relation to the form (2), where the movement of the shock wave front is determined by two-dimensional parameters: the explosion energy E and the initial density of the buffer gas ρ_g [12]:

$$\Psi(t)=\left(1+\frac{\xi_0}{R_0}\left(\frac{E}{\rho_g}\right)^{1/5}t^{2/5}\right)^2=\left(1+\alpha_0 t^{2/5}\right)^2,$$

$$\alpha_0 = \frac{\xi_0}{R_0}\left(\frac{E}{\rho_g}\right)^{1/5}, \quad \xi_0 = \left\{\frac{75(\gamma_g - 1)(\gamma_g + 1)^2}{16\pi(3\gamma_g - 1)}\right\}^{1/5}, \tag{2}$$

where γ_g – ratio of specific heat (adiabatic) of the buffer gas ($\gamma_g = \frac{7}{5}$, $\xi_0 = 1.014$).

Approximation (2) allows us to achieve a good correspondence with experimental data even without introducing fitting coefficients [13] (see fig. 1, dashed curve).

Model of spatial-temporal distributions of thermophysical parameters inside the silver ablation jet. The processes of dynamic condensation

In paper [12], it is proposed the model the spatial-temporal distributions of gas density inside the jet ρ and pressure P for the case of atmospheric gases. This model uses the degree of parabola up to 8 (provides a more real size of the transition zone from internal to external parameters) and obtain additional parameters that provide correct boundary conditions (density and pressure of atmospheric gases at the external boundary of the jet). As a result, we have the relations (3):

$$\rho(r, t) = \rho_0\left(1 - \xi^8\right)^{3/2}\left(1 + \alpha_0 t^{2/5}\right)^{-3} + \rho_g \xi,$$

$$P_P(r, t) = P_0\left(1 - \xi^8\right)^{5/2}\left(1 + \alpha_0 t^{2/5}\right)^{-5} + P_g \xi, \tag{3}$$

where $\xi = \frac{r}{R(t)}$ – dimensionless Lagrangian coordinate (inside the jet $0 \le \xi \le 1$), ρ_0 and P_0 – the density and pressure of vapor in the center of the jet at the initial moment, respectively, ρ_g and P_g – density and pressure of the buffer gas (air atmosphere), respectively.

Three-dimensional surfaces corresponding to the proposed space-time distributions of silver vapor pressure and density inside the jet are shown at the fig. 2.

According to the Zeldovich – Raiser theory [9], condensation must necessarily begin at some point during adiabatic expansion of vapor. This moment can be determined from the following considerations: on the phase diagram of the vapor states, its expansion occurs along the Poisson adiabate until the moment of saturation, i. e. until the intersection of the Poisson adiabate with the saturation adiabate given by the Clausius – Klayperon equation [9]. Further, continuing to follow the adiabate of Poisson, the vapor of the jet becomes supersaturated (supercooled), and conditions are created for the formation of nuclei of future drops. The rate of formation of condensation nuclei is exponentially dependent on the degree of vapor supersaturation, which is defined by

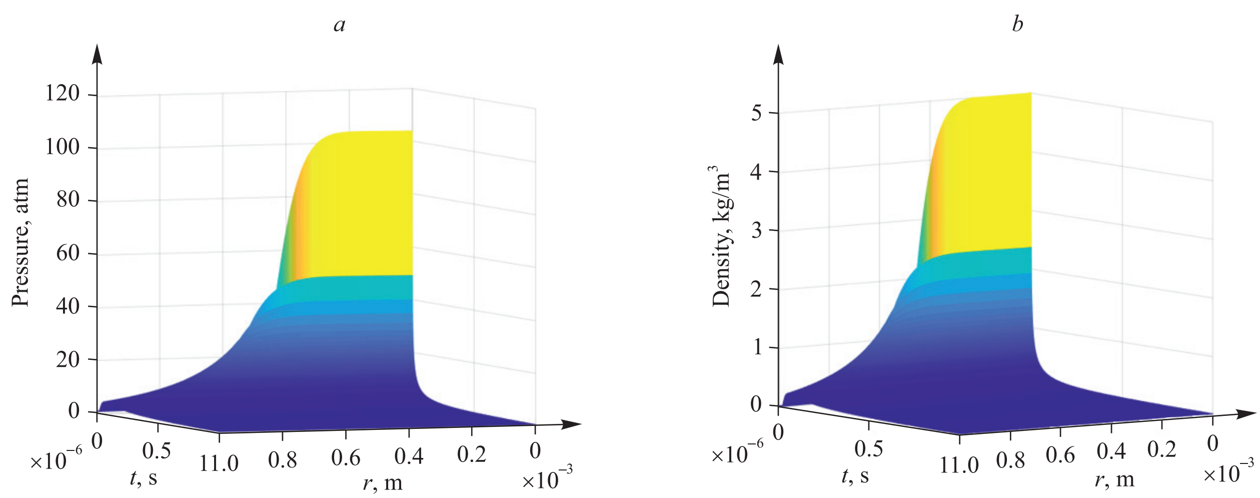

Fig. 2. Spatial-temporal distributions of pressure (*a*) and density (*b*) of silver vapor inside the jet

parameter of supercooling $\theta = \frac{T_{eq} - T}{T_{eq}}$, where T_{eq} is the temperature of the thermodynamic equilibrium for the given volume and pressure (temperature along vapor binodal line on the phase diagram separating stable and metastable states [8]).

Further, with a sharp increase in the degree of supersaturation of vapor, there is a bulk formation of condensation centers («etching» of nuclei), which due to the «sticking» of vapor molecules begin to grow in size. Accelerated formation of liquid drops in vapor due to the release of latent condensation energy stops the growth of the supercooling parameter and causes its decline. In this case, the process of nuclei formation, which is extremely sensitive to the degree of supersaturation, stops and in the future only the enlargement of the formed droplets occurs.

Due to the continued rapid expansion of the jet at this stage, gradual decrease in the number of acts of «sticking» of vapor molecules to the nuclei can be obtained, and subsequently we can observe their complete cessation. In this case, the degree of vapor condensation x (the ratio of the number of vapor atoms in the liquid phase to their total number) is stabilized, which corresponds to the so-called «quenching» of droplets [9]. Thus, in contrast to the equilibrium static condensation scenario, when the vapor is in a state of thermodynamic equilibrium at all stages, the maximum achievable degree of condensation in the case of rapid adiabatic expansion of the jet can be significantly less than 1 (in practice, $x = 0.1–0.3$ [4]).

The temperature dynamics in the center of the silver ablation jet ($\xi = 0$) is shown in fig. 3, *a*, where you can see these patterns. Initially, this parameter follows the Poisson adiabate and the value $T_c = 2901$ K corresponds to the moment when the Poisson adiabate intersects with the saturation adiabate. After reaching this value, the vapor becomes supersaturated and conditions for nuclei formation are created. The temperature in the jet center deviates from the Poisson's adiabate at the moment of bulk «etching» of nuclei (at $T_e = 1232$ K), corresponding to the maximum supercooling of vapor.

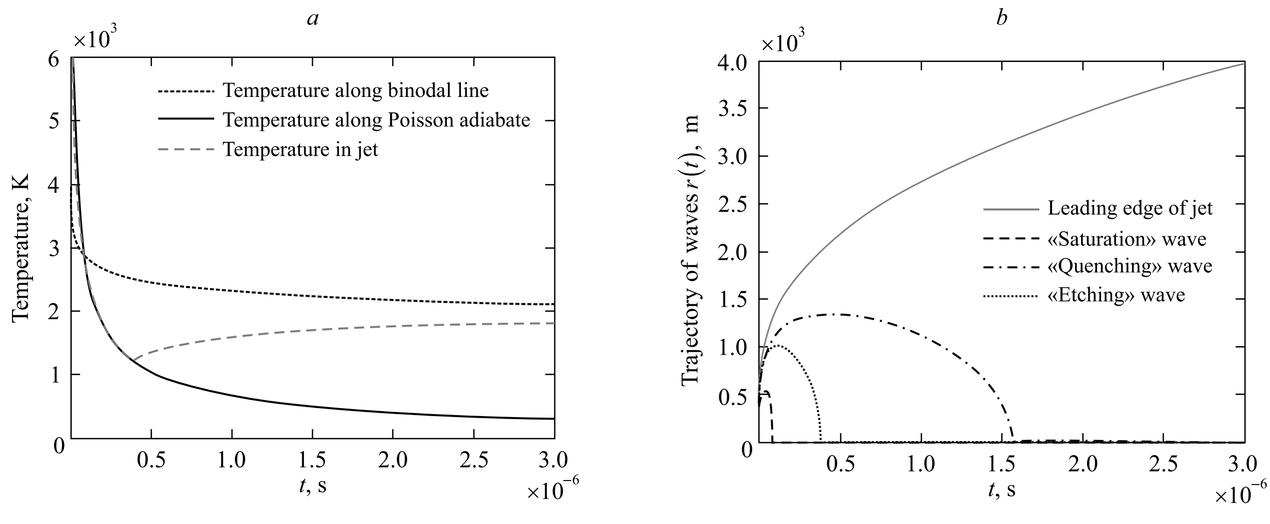

Fig. 3. Dynamic condensation in silver jets:
a – temperature dynamics in the center of the silver ablation jet ($\xi = 0$);
b – wave fronts of dynamic condensation

Described above process of dynamic condensation of silver ablative jets can also be graphically represented as passing of the three spatial concentric spherical waves in the expanding vapor-plasma cloud from the periphery to the center. There are «saturation» wave (corresponding to the moment of crossing the adiabatic Poisson curve with adiabatic saturation curve at the phase diagram of vapor), wave of nuclear «etching» (the moment of greatest supercooling) and the «quenching» wave (stabilization of the degree of condensation of the vapor) [4; 8]. To evaluate the spatial-temporal characteristics of the «saturation», «etching» and «quenching» waves, it is proposed to use the relations [8; 12] taking into account the jet expansion model (2):

$$r_c(t) = R_0\left(1 + \alpha_0 t^{2/5}\right)\sqrt{1 - \frac{T_c}{T_0}\left(1 + \alpha_0 t^{2/5}\right)^2},$$

$$r_e(t) = R_0\left(1 + \alpha_0 t^{2/5}\right)\sqrt{1 - \frac{T_e}{T_0}\left(1 + \alpha_0 t^{2/5}\right)^2},$$

$$r_q(t) = R_0\left(1 + \alpha_0 t^{2/5}\right)\sqrt{1 - \left(\frac{4}{5}t_k\left(1 + \alpha_0 t^{2/5}\right)^3 \alpha_0 t^{-3/5}\right)^{1/2}},$$
$$t_k = \frac{mV_0}{2\sigma_g}\sqrt{\frac{3m}{5k_B T_0}}, \tag{4}$$

where $r_c(t)$, $r_e(t)$, $r_q(t)$ – radiuses «saturation», «etching» and «quenching» waves, respectively; σ_g – cross section of the collision process; $V_0 = \frac{1}{\rho_0}$ – specific volume of the jet; m – molar mass of Ag; k_B – Boltzmann constant.

Figure 3, *b*, shows the trajectories of «saturation», «etching» and «quenching» waves in the ablation jet of silver, constructed in accordance with (4). It should be noted that the time scale of model waves is in good agreement with experimental data [13] even without introducing fitting coefficients.

Conclusion

This paper demonstrates the possibility of adapting the Anisimov – Luk'yanchuk model to describe the processes of droplet formation in ablative silver jets at atmospheric pressure. Despite some differences due to the presence of buffer gases in the jet propagation zone, the proposed approach gives a good agreement with the experimental data, even in the absence of fitting parameters. It allows you to predict the development of an ablative laser jets when such initial conditions as the initial internal energy of the jet and the pressure of the surrounding gas change. This plays an important role in the development of a new technological direction: controlled laser-induced deposition of surface metal nanostructures at atmospheric pressure [16–18].

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