GAS–DYNAMICAL MODEL OF HIGH–MELTING PARTICLE EVAPORATION IN A POWERFULL OPTICAL FIELD ALLOWING FOR RECONDENSATION IN VACUUM

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As is well known, the process of gas–dynamical evaporation of high–melting aerosol particles in a powerfull optical field in vacuum is accompanied by active condensation of vapors and formation of new particles. In this paper a thermodynamic method of estimating the vapor condensation ratio is discussed. Normally the system of gas–dynamical equations describing the vapor outflow is solved numerically, while in this paper an analytical solution of this system in quasistationary approach based on the isentropic character of the vapor outflow from the particle surface is obtained. The obtained results make it possible to formulate the problem of the determination of the optical cross section of the particle + condensate system.

When high–power optical radiation with an intensity of ~ 10^9 W/m^2 propagates through a disperse medium containing high–melting particles the latter can be heated up to the temperatures up to ~ 3000 – 5000 K.[1] At so high temperatures the pressure of saturated vapors of the aerosol particle substance is, as a rule, much higher than the atmospheric pressure. Under these conditions the separation of vaporizing substance from the particle surface takes place with a high speed that makes the diffusion model of vaporization inapplicable. A model of an isolated aerosol particle evaporation in the field of laser radiation, which enables one to calculate the speed of separation of fragments and the other thermodynamic characteristics of vapor in the medium with counter pressure, has been developed in Refs. 2 and 3. As was shown in Ref. 4, the vapor while moving from the surface of the particle, is rapidly cooled and becomes oversaturated. Hence it follows that the adequate model of a high–melting particle evaporation should allow for the vapor recondensation and formation of a cloud of secondary particles. Interaction of radiation with such disperse media can result in new nonlinear effect due to the recondensation because of the transformation of the optical properties of the system due to the formation of the secondary particles.

In this paper we study the model of interaction between the laser radiation and a separate immobile high–melting particle in vacuum which takes into account the formation of the secondary aerosol particles due to the vapor condensation. This model can be useful for the solution of the problem of determining the optical cross section of the particle + condensate system.

Let us assume that a spherical aerosol particle of radius a is placed in the field of laser radiation and is heated up to the temperature T_s. It is clear that the temperature of the particle surface is determined by the radiant flux density, optical properties of the evaporating particle, and, of course, by the energy losses due to evaporation and reemission. However, at this stage we assume the temperature of the particle surface to be preset. In this case the gas–dynamical equations describing the separation of the substance evaporated from the particle surface can be written as follows:

$$\frac{\partial\rho}{\partial t} + \mathrm{div}(\rho v) = 0\ ,$$

$$\frac{\partial v}{\partial t} + (v,\ \Delta)\ v + \frac{1}{\rho m_0}\ \mathrm{grad}\ P = 0\ . \qquad (1)$$

Here $\rho = \rho(t,\ r)$ is the number density of atoms or molecules of the evaporated substance, r is the distance from the particle center to the point of observation, $v = v(t,\ r)$ is the speed of the vapor separation, m_0 is the mass of atom or molecule, and $P = P(t,\ r)$ is the vapor pressure.

Note that the molecules of the evaporating substance can be both in the gaseous and in the condensed (either solid or liquid) phases. If the vapor condensation ratio is defined as

$$x(T) = \frac{\rho_c}{\rho_g + \rho_c} = \frac{\rho_c}{\rho}\ , \qquad (2)$$

where ρ_c is the number density of molecules in a condensed phase and ρ_g is the number density of molecules in the gas phase, then we have $\rho_c = x\rho$ and $\rho_g = (1 - x)\rho$.

Characteristic relaxation time of the thermodynamic parameter fields $t \sim a/v \sim 10^{-8}$ s for $a \sim 10$ μm and $v \sim 1000$ m/s. At the same time the characteristic time of the particle size change due to its evaporation is of the order of $t_{ev} \sim 10^{-4}$ s according to Ref. 3. As a consequence, the radius of the particle varies only slightly in the course of the field relaxation. Therefore, Eqs. (1) can be solved in a quasistationary approach, according to which all thermodynamic characteristics of the vapor depend on time only parametrically via slowly varying boundary conditions. In the quasistationary approach the temperature of different points of the particle surface is practically identical, though the particle is heated up by the laser radiation only from one side.[5] Taking this into account and neglecting the initial quite short time interval from the start of the laser action we can solve this problem assuming the spherical symmetry.

In this case Eqs. (1) take the form

$$\frac{1}{r^2}\frac{d}{dr}(r^2\rho v) = 0\ ;$$

$$\frac{1}{\rho m_0}\frac{dP}{dr} + v\frac{dv}{dr} = 0\ . \qquad (3)$$

The system (3) is open. It can be closed in two ways corresponding to two different regimes of the vapor outflow.

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1. In the region where the vapor is supersaturated we can assume the process of the vapor expansion to be adiabatic and then we have $P = \alpha\rho^{\gamma}$, where α is the constant determined from the boundary conditions and γ is the adiabatic exponent.

2. In this regime the vapor is saturated or supersaturated. In this case there exists a relatively small region[4] where the supersaturation ratio differs from unity. The supersaturation ratio δ in the region of intense nucleation is about 10^3 (estimates of this value are given below). Out of this region the vapor expansion follows the adiabat of the two–phase system, the supersaturation ratio is equal to zero, and the excess of vapor is condensed on the previously formed condensation nuclei. The pressure of vapor in this region is equal to the pressure of saturated vapor. We consider the latter to be a well–known function of temperature[6]

$$P_s = P_\infty \exp(-L/kT) , \tag{4}$$

where T is the temperature of vapor in the field of observation , L is the heat of evaporation of one atom of particle substance, k is the Boltzmann constant, and P_∞ is the factor of dimensionality. Then using Eq. (2) we obtain

$$\rho = \frac{P_\infty \exp\left(-L/kT\right)}{(1-x)\,kT} , \tag{5}$$

where the unknown temperature can be determined from the condition

$$T = \frac{L}{k \ln P_\infty/P} . \tag{6}$$

The relations (4)–(6) together with Eq. (3) could make a closed system of equations if the function $x(T)$ were known.

The number of vapor molecules colliding with the surface of a secondary particle per second is $dN/dt \sim \rho\cdot\bar{v}\cdot a_{sp}^2$. It then follows that the radius of the secondary particle will change with rate

$$\frac{da_{sp}}{dt} \sim \frac{m_0\rho}{\rho_{sp}}\bar{v} ,$$

where a_{sp} is the radius of the secondary particle, $\bar{v}$ is the mean thermal velocity of the vapor molecules, and ρ_{sp} is the density of the secondary particle substance. Note that the values ρ and ρ_{sp} have different dimensionalities (see formula (1)). Then the characteristic time of the secondary particle radius change is

$$\tau \sim \frac{a_{sp}\rho_{sp}}{m_0\,\rho\bar{v}} .$$

Let us now estimate this time and the size of the region in which the formation of secondary particles occurs.

At temperature $T \sim 10^3$ K the vapor pressure is close in value to the atmospheric one hence $m_0\rho \sim 1$ kg/m^3. As is well known (see Ref. (7)), $a_{sp} \sim 10^{-9}$ m, then $\tau \sim 10^{-9}$ s. The size of the region where the formation of the nucleation centers takes place is $d \sim \bar{v}\tau \sim 10^{-6}$ m, and the characteristic time of the vapor expansion from the particle surface is $a/\bar{v} \sim 10^{-8}$ s. Therefore, in the first–order approximation we can assume that all the excess vapor is instantaneously condensed on the nucleation centers formed within a small region and the vapor is in thermodynamic equilibrium with the condensed phase. In this approach the condensation ratio can be found using thermodynamic methods.

Let us now consider a small volume V containing the constant number of atoms N_0. Let this volume move from the particle together with the flow of vapor, which is composed of saturated vapor and condensate.

Assuming the expansion of this volume to be adiabatic, we have

$$dU + PdV = 0 , \tag{7}$$

where

$$dU = \left(\rho_2 VC_g + \rho_c VC_c\right) dT - Ld\,(\rho_c V) . \tag{8}$$

Here dU is the variation of the internal energy of the two–phase (vapor + C–phase) system within the volume V being studied. C_c and C_g are the specific heat per atom of the C–phase and the gas, respectively.

Using the definition of the function $x(T)$ we can write the relation for the elementary work

$$\delta A = PdV = -kT\left(Vd\rho_g + N_0 dx\right) = k(1-x)(L/kt - 1)\,dT + dx. \tag{9}$$

Within the frameworks of the above approximations $P = P_s(T)$ we have

$$P = P_\infty \exp(-L/kT) . \tag{10}$$

On account of Eqs. (8) – (10) and after simple transformations Eq. (7) takes the form (in dimensionless units)

$$\frac{dx}{d\theta} = \frac{1}{\theta}\,\frac{\tilde{C} - (1-x)(\tilde{L}/\theta - 1)}{\tilde{L}/\theta + 1} , \tag{11}$$

where $\theta = T/T_s$, $\tilde{L} = L/kT_s$, $\tilde{C} = (C_c\cdot x + (1-x)\cdot C_g)/k$. Equation (11) with the initial conditions $x = 0$ and $T = T_c$, where T_c is the temperature of the medium at the point where the vapor pressure is equal to that of saturated vapor, can be solved numerically. If the vapor near the particle surface is saturated, then $T = T_s$.

In the case of the carbon particle evaporation, $L = 1.19\cdot10^{-18}$J/atom and $T_s = 5000$ K and the inequality $\tilde{L}/\theta > 1$ is always valid. As a result, Eq. (11) can be written in the form:

$$\frac{dx}{d\theta} = \frac{\tilde{C}}{\tilde{L}} - \frac{1-x}{\theta} . \tag{12}$$

Estimation of the order of the quantities in the right side of Eq. (12)

$$\tilde{C}/\tilde{L} \sim kT_s/L \sim 10^{-2},\ \frac{1-x}{\theta} \sim 1 ,$$

show that the first term of this equation can be neglected. The equation with the above–indicated initial conditions

$$\frac{dx}{d\theta} = -\frac{1-x}{\theta} \qquad (13)$$

can be easily solved analytically.

Figure 1 presents the function $x(\theta)$ obtained by numerical solution of Eq. (11).

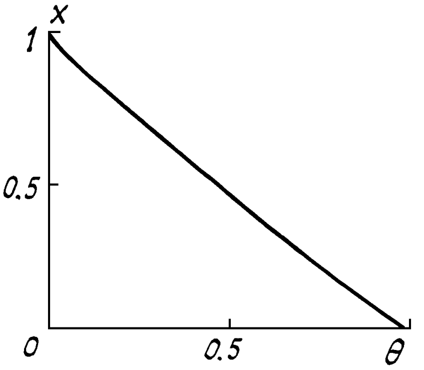

FIG. 1. The carbon vapor condensation ratio as a function of T/T_s at T_s = 5000 K.

It follows from Eq. (11) that as $\theta \to 0$, $x \to 1$. This, in fact, is a natural consequence of the thermodynamic method. However, in practice, certain portion of the particle substance in the gas phase volatilizes in gaseous phase. The extreme value of the condensation ratio x_{ex} can be estimated as the value of $x(\theta)$ at the point in which the free path became approximately equal to the size of the aerosol particle and the thermodynamic equilibrium is not established.

Thus, within the framework of the above approach, the closed system of equations in the region of condensation takes the form

$$\frac{1}{r^2}\frac{d}{dr}(r^2\rho v) = 0\ ; \qquad (14)$$

$$\frac{1}{\rho m_0}\frac{dP}{dr} + v\frac{dv}{dr} = 0\ ; \qquad (15)$$

$$\rho = P/\{(1-x)\,kT\}\ ; \qquad (16)$$

$$T = L/(k\ln P_\infty/P)\ ; \qquad (17)$$

$$x = 1 - T/T_c\ . \qquad (18)$$

Boundary conditions for this system are prescribed on the particle surface and have the form[8]

$$\rho_0 = 0.31\rho_s\ ; \qquad (19)$$

$$x_0 = 0\ ; \qquad (20)$$

$$v_0 = c = \sqrt{\frac{5kT_0}{3m_0}}\ ; \qquad (21)$$

$$T_0 = 0.65T_s\ . \qquad (22)$$

Prior to the vapor condensation, the system (14) – (18) with the boundary conditions (19) – (22) can be solved analytically.

Taking into account the law of conservation of the evaporating substance flow

$$j = 4\pi r^2\rho v = \text{const} \qquad (23)$$

and assuming the evaporation process to be adiabatic, we can write, after some transformations, Eq. (15) in the form

$$\frac{d\rho}{dr} = \frac{\rho}{r}\,\frac{2(v/c)^2}{1-(v/c)^2}\ , \qquad (24)$$

where $c = \sqrt{\frac{5kT}{3m_0}}$ is the local speed of sound. As is well known, Eq. (24) describes two regimes of evaporation, i.e., the subsonic and supersonic ones.

In the subsonic regime the initial rate of evaporation is lower than the speed of sound and, as can be seen from Eq. (24), $d\rho/dr > 0$. As a consequence, the density of vapor increases with distance from the surface of evaporating particle. It is clear that in the case of evaporation in vacuum this regime contradicts the condition $\rho(\infty) \to 0$. In the supersonic regime $d\rho/dr < 0$ and the density of vapor decreases with distance from the particle center.

In the case of the carbon particle evaporation it can be seen from Eq. (19) that already on the particle surface the vapor is supersaturated. In fact, the condensation of vapor starts in a small region near the particle surface (the size of this region has been determined above) and the quantity x here differs from zero. At the same the temperature of the two–phase system increases from $T = 0.65\ T_s$ up to T' as a result of time the release of the latent heat of condensation due to formation of the C–phase. This means that from the very beginning of the condensation process new boundary conditions are needed.

Assuming that out of this region the density of vapor is equal to that of saturated vapor, we can rewrite the boundary condition (19) in the form

$$\rho_{r0}(T') = \rho_s(T') = \frac{P_\infty}{kT_s}\exp\left(-L/kT'\right)\ . \qquad (25)$$

On account of Eqs. (19) and (25), we can write the following relation for the supersaturation ratio with such a discontinuity of the evaporating substance density

$$\delta = \frac{P - P_s}{P_s} = \frac{0.31\exp\left(-L/kT_s\right)}{\exp\left(-L/0.65T_s k\right)} - 1\ ,$$

At temperature T_s = 5000 K δ is on the order of 10^3.

Using the definition of the condensation ratio and taking into account Eqs. (19) and (25) we can estimate x at the temperature T' as follows:

$$x(T') = \frac{\rho_0 - \rho_{r0}(T')}{\rho_{r0}(T')}\ . \qquad (26)$$

The speed of vapor separation in this region is assumed to be equal to the sound speed in gas and the boundary condition (21) remains unchanged.

Thus, taking into account Eqs. (21) and (26), we can write new boundary conditions for the system of gas–dynamical equations (14) – (18) in the form

$$\rho'_{r0} = \rho_s(T')\ ;\ \ x_0 = \left(\rho_0 - \rho'_{r0}\right)/\rho'_{r0};\ \ v_0 = c\ . \qquad (27)$$

Unknown temperature T' in Eq. (27) will be determined below and, therefore, this system of boundary conditions becomes closed.

Assuming that the expansion of a gas in vacuum is an isentropic process, we can solve Eqs. (14) and (15) with boundary conditions (27) analytically.

Transforming Eq. (15) to a form

$$\frac{d}{dr}\left(\frac{m_0 v^2}{2}\right) + V\frac{dP}{dr} = 0 \tag{28}$$

and using the well–known thermodynamic relations for energy and enthalpy of the system

$$dE = TdS - PdV,\ \ dW = d(E + PV)\ ,$$

as well as taking into account Eq. (7) we find that $V\,dP = dW$. In this case Eq. (28) takes the form

$$\frac{d}{dr}\left(\frac{m_0 v^2}{2} + W\right) = \frac{dW'}{dr} = 0\ . \tag{29}$$

$$W' = (1 - x)\,C_p T + C_c x T - Lx + \frac{m_0 v^2}{2}\ , \tag{30}$$

where C_p is the specific heat of the gas at constant pressure.

The boundary condition for W'_0 by virtue of Eqs. (21) and (22) will take the form

$$W'_0 = C_p T_0 + \frac{m_0 c^2}{2}\ . \tag{31}$$

Let us find the boundary condition for the temperature of the two–phase system. Since the value W' remains constant and is equal to W_0, we obtain the following expression for the temperature of the two–phase system:

$$T' = \frac{C_p T_0 + Lx}{C_p(1 - x) + C_c x}\ . \tag{32}$$

In order to find the values of the condensation ratio and temperature T' of the gas, we must solve the system of two algebraic equations (26) and (32). Inverting and making log–to–linearization of Eq. (32), we obtain

$$T' = \frac{L}{k\,(\ln A + x)}\ , \tag{33}$$

where

$$A = 1/\left[0.31\,\exp\left(-L/kT_s\right)\right]\ .$$

Solving simultaneously Eqs. (32) and (33) we find that $x'_0 = 0.04$. Then $T' = 4672$ K. On account of these values, new boundary conditions take the form

$$\rho'_{r0} = \rho_s(T')\ ;\ x'_0 = 0.04\ ;\ v_0 = c\ ;\ T' = 4672\ . \tag{34}$$

Provided that $x(T)$ is well–known, we obtain from Eq. (30) the following relation for the vapor separation speed:

$$v = \sqrt{\frac{2}{m_0}\left(W'_0 - \left((1 - x)C_p T + C_c x T - Lx\right)\right)}\ . \tag{35}$$

On the other hand, it follows from the law of conservation of the evaporating substance flow that

$$v = j/4\pi r^2 \rho = \frac{j(1 - x)kT_s}{4\pi r^2 P_\infty e^{-L/kT}}\ , \tag{36}$$

where j can be determined from boundary conditions (34). By expressing r from Eq. (36)

$$r = \sqrt{\frac{j(1 - x)\,kT_s}{4\pi P_\infty e^{-L/kT} v}}$$

and taking into account that the function $x(T)$ is well known, we can determine the fields of pressure, temperature, and density of vapor in the vicinity of the particle.

The calculations of the fields of temperature, pressure, and density of vapors in the vicinity of the particle with the radius $a = 100$ μm at surface temperature 5000 K have been made in this paper both analytically and numerically.

The analytical and numerical results are practically identical in the scale used in this paper for the figures. In fact the difference between so–obtained results is 5 – 10 %. Based on this fact we can state that the method enables one to determine the thermodynamic characteristics of the system without numerical solution of the gas–dynamical equations.

Figure 2 shows the dependence of the speed of vapor separation on the reciprocal distance from the primary particle. It can be seen from this figure that the separation speed increases for the entire interval of values r.

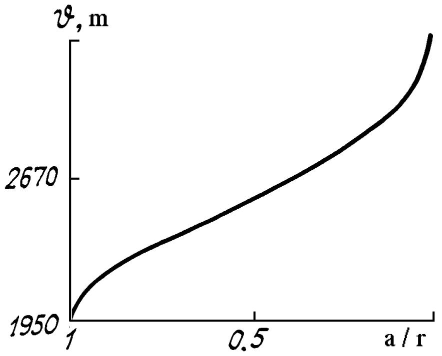

FIG. 2. The separation speed of carbon vapor as a function of the reciprocal distance from the primary particle for $a = 100$ μm *at* $T_s = 5000$ K.

Figures 3 and 4 show the dependences of temperature and condensation ratio of the vapor on the reciprocal distance, respectively. One can see from Fig. 4 that for $r \sim 10\,a$ the condensed phase contains ~ 25% of the evaporated substance. Since in this region the free path is comparable with the size of particle, while the separation speed of vapor is much higher than the local sound speed, the fine fraction have no time to grow up and, as a consequence, certain portion of substance leaves the particle being in the gaseous state.

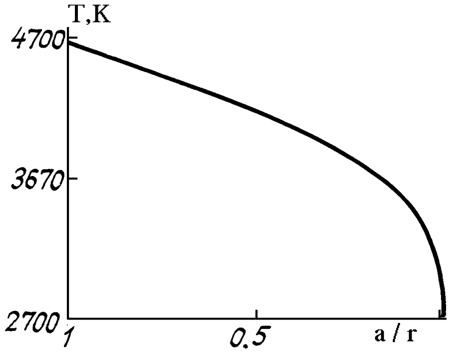

FIG. 3. Temperature of carbon vapor as a function of the reciprocal distance from the primary particle for $a = 100$ μm *at* $T_s = 5000$ K.

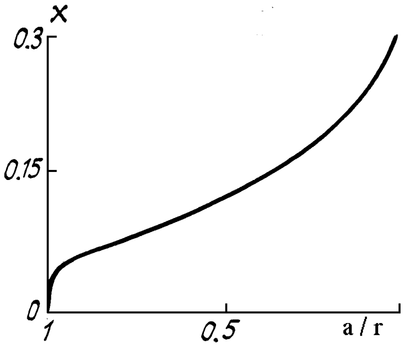

FIG. 4. The condensation ratio of carbon vapor as a function of the reciprocal distance from the primary particle for $a = 100$ μm *at* $T_s = 5000$ K.

CONCLUSIONS

The proposed model of a high–melting particle evaporation in vacuum allowing for the recondensation process makes it possible to determine the characteristics of the two–phase system, including the size distribution function (SDF) of secondary particles.

It is obvious from the physical point of view that the SDF of the particles contained in any spherical layer is the δ – function of the form $n(r)\,\delta(a - a(r))$, where $n(r)$ is the number density of particles being dependent of the distance r due to the changes in the geometry of the expanding volume of substance and $a(r)$ is the function of the particle size.

As a result one can calculate, using this model, the value of light scattering cross section of the two–phase system

$$\sigma = \int\limits_0^\infty \kappa_a(a)\, \pi a^2(r)\, n(r)\, 4\pi r^2\, dr ,$$

where $\kappa_p(a)$ is the scattering absorption efficiency of the particle with radius a.

Simple estimations of the scattering cross section yield

$$\sigma \approx \kappa_a(a)\pi\, \overline{a^2}\, N ,$$

where N is the number of secondary particles with mean radius $\overline{a}$ contained in the spherical layer whose radius can be found from the condition of complete evaporation of the primary particle. Thus, for a particle with radius $a = 10$ μm the scattering cross section $\sigma \sim 10^{-8}$ m^2.

However more exact calculations of the scattering cross section of the two–phase system and more correct conclusions require the knowledge of $n(r)$ and $a(r)$ functions as well as more comprehensive analysis.

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