Metallic melt fracture and fragmentation under the high-current electron irradiation

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Abstract Action of the high-current electron beam leads to an intensive heating of a surface layer of the irradiated metal. Rapid temperature increase can cause melting of the surface layer and generate intensive stresses in it. Release of these stresses induces fast expansion of the molten metal and, on the contrary, results in tension. Tension of the melt activates nucleation, growth and coalescence of vapor bubbles, it means, fracture and fragmentation of the metallic melt. In present work we numerically investigate kinetics of the liquid metal fracture and fragmentation under the dynamic tension initiated by the powerful electron irradiation. Metal is treated as a two-phase medium consisting of vapor bubbles in liquid metal at the first stage of the evolution and of liquid drops in vapor at the second stage. Two-level approach is used: on the macroscopic level, the irradiated metal is treated as a two-phase heterogeneous medium in the one-velocity approximation, while on the microscopic level, the exchange of energy, mass and volume between both phases are described including grow or decrease of size of the vapor bubbles or liquid drops. Generation of ultra-dispersed particles of copper at the high-current electron beam irradiation is numerically investigated.

Keywords Liquid metal, Dynamic fracture, Electron irradiation, Heterogeneous medium, Vapor bubbles

1. Introduction

Action of the high-current electron beam on the metals can be used for production of the ultrafine metal particles [1,2]. The process of particles formation passes through several stages. At the first stage, during the irradiation, fast beam electrons lose their energy in the substance, which leads to the metal heating and formation of the high pressure region inside the energy release zone [3-5]. The next stage is an expansion of the heated and "compressed" layer of metal, which generates tensile stresses (negative pressure) in it. Destruction of the expanded metal begins at the expense of nucleation and growth of cavities. The higher temperature of the surface layer leads to the lower threshold of the negative stress, required for the destruction [6,7].

Complete destruction of the liquid phase takes place when the cavities grow up thus much to coalescence with each other forming a singly connected vapor phase, while the remaining liquid is fragmented on drops. The following expansion of the vapor-drops mixture (aerosol) is accompanied by the metal evaporation and condensation on drops. At the sufficient level of the enclosed energy, the liquid drops can be fully evaporated with formation of pure vapor. In turn, the adiabatically expanding vapor can become oversaturated, which result in the nucleation of liquid drops in it. In the paper [8] the condensation of the metal particles from the pure vapor, obtained at the complete evaporation under the action of the high-current electron beam, was numerically investigated; it was shown, that the homogeneous nucleation and the coagulation of the drops determine the size of the produced metal nanoparticles.

Meanwhile, the electron beam irradiation leads to the incomplete evaporation in the most cases. A part of metal remains condensed in the form of liquid drops. During the adiabatic expansion these drops become the centers of condensation; their quantity determines the quantity and size of the formed ultrafine metal particles. In this report a mathematical model of the ultrafine metal particles formation in the case of incomplete evaporation is described. Kinetics of evaporation and condensation of metal irradiated by the high-current electron beam is numerically investigated.

Metastable version of the wide-range equations of state [9,10] has been used for the description of superheated liquid and supersaturated vapor.

2. Mathematical model of substance dynamics with evaporation and condensation

Metal was treated as a two-phase medium consisting of the vapor bubbles in liquid metal on the first stage and of the liquid drops in vapor thereupon. Size of bubbles and drops (about $0.1\ \mu\text{m}$) is less than the typical length scale of the problem (the last one is of the order of electron rage in substance about $10 \div 1000\ \mu\text{m}$). It allows using of the continuous approximation in which both phases are described by continuous fields of parameters: concentration and radius of bubbles (drops), pressure, temperature, density and volume fraction of liquid and vapor phases in each point of space. Estimations showed that the phases must have approximately the same velocities; therefore we have used a one-velocity approximation. Substance dynamics has been described by the continuum mechanics equations. The beam action has been taken into account through energy release of fast electrons. Generation and growth of vapor bubbles and consequent evolution of drops have been described by kinetic equations for phase transition [11]. A simple scheme of transition from the bubbles in liquid to the drops in vapor (a percolation problem) has been constructed.

We consider the 1D problem: substance moves along z-axis. At different stages of evolution the medium means: a) pure condensed metal (solid or liquid); b) liquid metal with trapped bubbles; c) vapor with trapped drops; and, maybe, d) pure vapor. The liquid (or solid) is a carrying agent at stages a) and b), while the vapor is carrying agent at stages c) and d). A dispersed phase consists of vapor bubbles at stage b) and of liquid drops at stage c); and this phase is clearly absent at stages a) and d).

The continuum mechanics equations for substance dynamics in Lagrangian coordinates are the next:

$$\frac{1}{\rho}\frac{d\rho}{dt} = -\frac{\partial v}{\partial z}, \tag{1}$$

$$\rho\frac{dv}{dt} = -\frac{\partial P_c}{\partial z}, \tag{2}$$

$$\rho\frac{dU}{dt} = -P_c\frac{\partial v}{\partial z} + \rho\cdot D, \tag{3}$$

where v is the z-component of substance velocity; P_c is a pressure in the carrying agent phase; D is the energy release function. Here and further the index c denotes the carrying agent phase, while the index d denotes the dispersed phase. Average density of the medium is $\rho = \rho_c\alpha_c + \rho_d\alpha_d$, where $\alpha_{c,d}$ is the volume fraction of corresponding phase. Average specific internal energy U is given by the next expression: $U = \left(U_c\alpha_c\rho_c + U_d\alpha_d\rho_d\right)/\rho$.

Eq. (2) determines the substance velocity v, which is equal for both phases. Eq. (1) and Eq. (3) must be supplemented by several assumptions for determination of the thermodynamic parameters of each phase. We have supposed that the dispersed phase volume is constant during the substance movement as a whole, and it changes only as a result of interaction between the phases; this interaction leads to the bubbles and drops growth or reduction. In these assumptions one can obtain the next equations:

$$\frac{d\alpha_c}{dt} = \alpha_d \frac{\partial v}{\partial z} - w, \tag{4}$$

$$\frac{d\alpha_d}{dt} = -\alpha_d \frac{\partial v}{\partial z} + w, \tag{5}$$

$$\frac{d\rho_c}{dt} = \frac{\rho_c}{\alpha_c}\left(-\frac{\partial v}{\partial z} + w\right) - \frac{J}{\alpha_c}, \tag{6}$$

$$\frac{d\rho_d}{dt} = -\frac{\rho_d}{\alpha_d} w + \frac{J}{\alpha_c}, \tag{7}$$

$$\rho_c \alpha_c \frac{dU_c}{dt} = P_c\left(-\frac{\partial v}{\partial z} + w\right) - Q, \tag{8}$$

$$\rho_d \alpha_d \frac{dU_d}{dt} = -P_c \cdot w + Q. \tag{9}$$

In the Eqs (4)-(9) w is the growth rate of the dispersed phase volume in a unit volume of the medium; it can be expressed as that follows:

$$w = n \cdot 4\pi R^2 \cdot \dot{R} + \left(4\pi/3\right) R_{cr}^3 \cdot \dot{n}, \tag{10}$$

where n is the concentration of the dispersed particles (bubbles or drops) in the medium, and R is radius of this particles; R_{cr} is the radius of critical (nucleating) bubbles.

In the Eq. (6), Eq. (7) J is the growth rate of the dispersed phase mass in a unit volume of substance:

$$J = n \cdot m_1 \cdot \dot{g} + \left(4\pi/3\right) R_{cr}^3 \cdot \rho_v \cdot \dot{n}, \tag{11}$$

where m_1 is the mass of one atom of the substance; g is a number of atoms in the bubble (or in the drop); ρ_v is a saturated vapor density. And, finally, the value Q characterizes the heat exchange between the phases, which tends to equal temperatures of the phases.

The next equation describes the bubbles growth in the liquid at the stage b) and a size change of the liquid drops at the stage c):

$$\ddot{R} = -\frac{3}{2}\frac{\dot{R}^2}{R} + \left[P_d - P_c - \frac{2\sigma}{R}\right] \cdot \frac{1}{R\rho} A - B\frac{8}{3}\frac{\eta}{\rho_c}\frac{\dot{R}}{R^2}, \tag{12}$$

where s is the surface tension and h is viscosity of the liquid metal; A and B are the numerical factors: $A = B = 1$ at the stage b), and $A = 5$, $B = 1,25$ at the stage c). Critical radius of the vapor bubble is equal to

$$R_{cr} = \frac{2\sigma}{P_v - P_c}, \tag{13}$$

where P_v is a saturated vapor pressure. The bubbles nucleation rate is

$$\dot{n} = \frac{c}{\left(2R_{cr}\right)^4} \cdot \exp\left(-\frac{W_{cr}}{kT_c}\right), \tag{14}$$

where c is a sound speed in liquid metal, T_c is a temperature, k is the Boltzmann constant, and is the formation work of the critical bubble:

$$W_{cr} = \frac{16\pi}{3}\frac{\sigma^3}{\left(P_v - P_c\right)^2}. \tag{15}$$

In the case of liquid drops, the condition $\dot{n} = 0$ has been supposed to hold, but the drops can

disappear if the number of atoms in it $g \le 2$ (the complete evaporation).

Number of atoms in each bubble is controlled by the next equation:

$$\frac{dg}{dt} = g\frac{2R}{c}\left[\exp\left(\ln\left\{\frac{P_v}{P_c}\right\} - \frac{4\pi R_1^2\sigma}{3kT_c \cdot g^{1/3}}\right) - 1\right], \tag{16}$$

where

$$R_1 = \left[\left(3m_1\right)/\left(4\pi\rho_v\right)\right]^{1/3}. \tag{17}$$

Pressure and temperature of the caring agent phase and of the dispersed phase have been obtained from the metastable equation of state: $P_{c,d} = P\left(\rho_{c,d}, U_{c,d}\right)$, $T_{c,d} = T\left(\rho_{c,d}, U_{c,d}\right)$. This equation of state has been used for determination of the density ρ_v and pressure of the saturated vapor as well.

Than the bubbles became large enough they merge and form a simply connected phase. On the contrary, the liquid divides on separate drops. These drops are the condensation centers in the expanding and cooling vapor. Number and sizes of the liquid drops are determined by the number and sizes of the vapor bubbles at the moment of merging. We have established this connection in a simplest case of equal distance between the bubbles centers. Bubbles merge then their diameters $2R$ reach the value of a distance between their centers. Single bubble occupy the volume $4\pi R^3/3$, liquid volume per one bubble at this time is $\left(8 - 4\pi/3\right)R^3$. We have assumed that the number of resulting drops is equal to the number of vapor bubbles, and then $\left(8 - 4\pi/3\right)R^3$ is the volume of one liquid drop. Due to the surface tension, the drops obtain a spherical form after the liquid phase division, and the radius of such spherical liquid drop can be estimated as $R_{\mathrm{L}} = \left(6/\pi - 1\right)^{1/3} R \approx R$. It follows, that the merging passes then the vapor volume fracture achieves the value $\alpha_c \approx 0.5$. A number of smaller drops can be formed during the vapor bubbles merging, but we neglect it here.

3. Numerical investigation of the metal fracture

We have numerically investigated the copper irradiation by the high-current pulsed electron beam with parameters: the energy of fast electrons is 1 MeV, the beam current density is 10 kA/cm^2, the pulse duration is 50 ns. The beam action causes the sharp heating of the substance (up to 4900 K) in the energy release zone (Fig. 1) and the formation of area of the high-pressure - up to 17 GPa (Fig. 2). The substance temperature exceeds the melting temperature up to the depth of 0.4 mm; in this layer the metal is melted. Release of the high pressure area results in formation of the compression wave with the amplitude up to 11.5 GPa. The compression wave front is becoming sharper with the time, and it transforms into the shock wave. Reflection from the free (irradiated) surface forms the rarefaction wave, following behind the shock wave. This rarefaction wave creates in the liquid metal the negative stress with the value up to 2.5 GPa, which initiates the fracture of the liquid phase through the generation and growth of the vapor bubbles. The generation and growth of the bubbles result in reduction of the liquid metal volume and, therefore, it releases the tensile stresses; the substance passes in the equilibrium two-phase state. This process restricts the tensile stresses; otherwise, the rarefaction wave amplitude would be the same as the amplitude of the compression wave.

It should be noted that the existence of metastable liquid state leads to propagation of the rarefaction (tensile) wave inside the metal behind the shock wave. Negative stresses in the rarefaction wave can reach 2.5 GPa. Thus, the structure of stresses in the metal differs from that in calculations [4,8],

where an approximation of the equilibrium two-phase state of the liquid and vapor was used for the description of the melted layers of metals. The rarefaction wave can substantially influence on the material modification [12] as well as on the spall fracture of solid metal near its back surface.

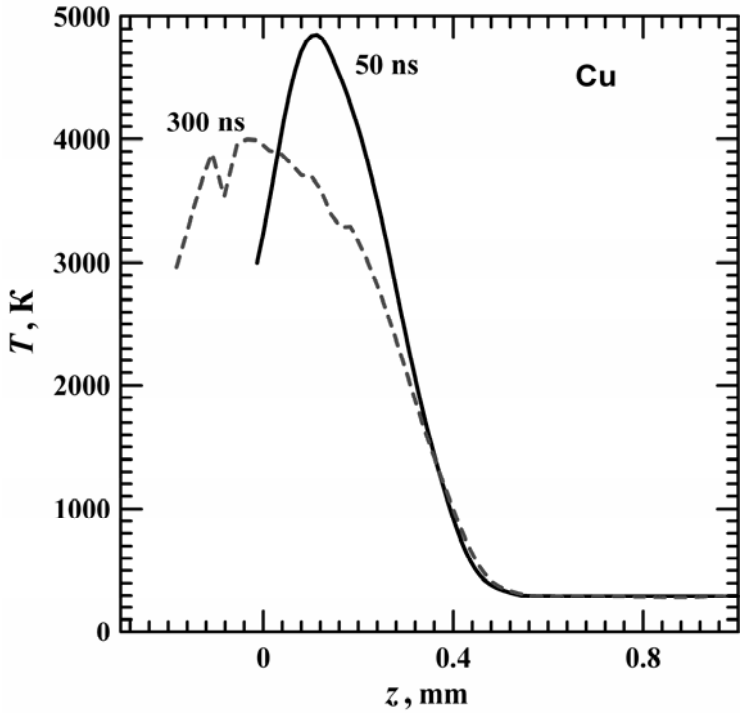

Figure 1. Temperature distributions in copper at the two time moments. Fast electrons energy is 1 MeV, the current density is 10 kA/cm^2, the pulse duration is 50 ns. At the moment of the pulse end, the temperature in the metal layer heated by the beam is maximal and it achieves 4900 K, after than, at the expansion of the "compressed" substance, the temperature becomes lower.

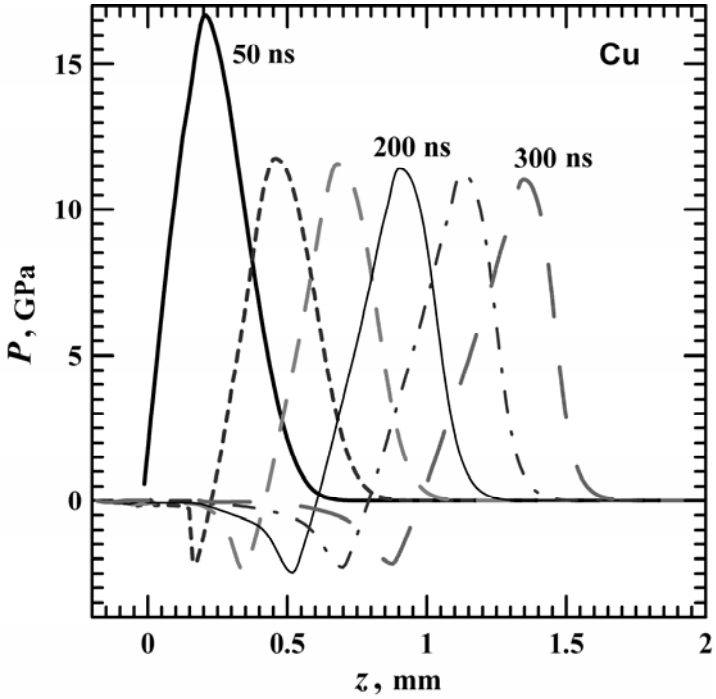

Figure 2. Distributions of pressure at consecutive time moments. High current electron beam irradiation of copper with the electrons energy 1 MeV, the current density 10 kA/cm^2, and the pulse duration 50 ns.

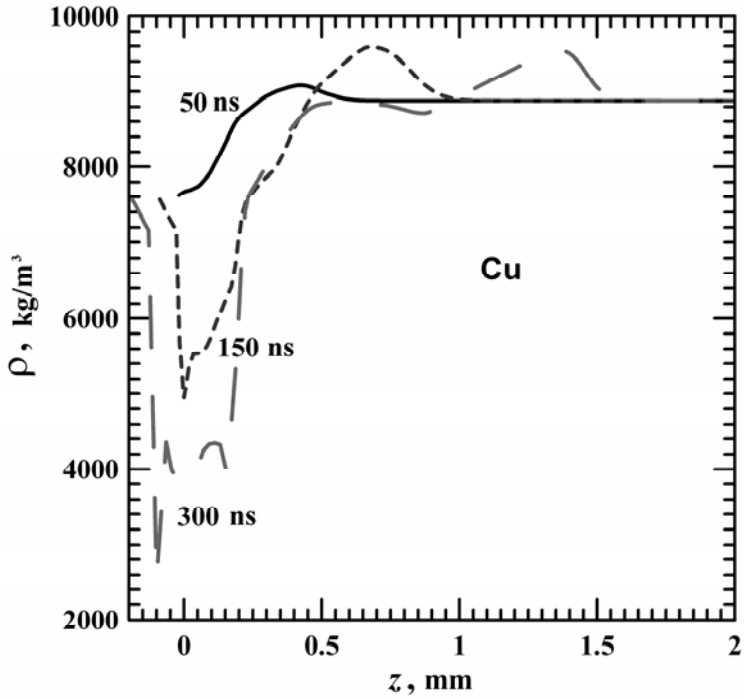

Figure 3. Distributions of the average density of the medium at consecutive time moments. High current electron beam irradiation of copper with the electrons energy 1 MeV, the current density 10 kA/cm^2, and the pulse duration 50 ns.

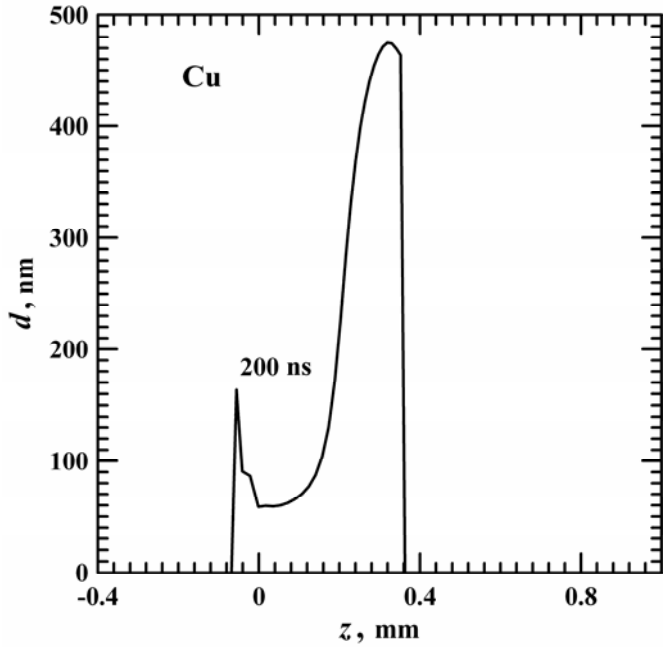

Figure 4. Depth distribution of the vapor bubbles diameters at the moment just before the fragmentation of the liquid phase. The lower bubbles diameters and, consequently, the larger concentrations correspond to the central region of the energy release zone, in which the tension occurs with the higher strain rate. Zero level corresponds here to the absence of the bubbles.

Appearance of the bubbles leads to the decrease of the average density of the two-phase medium (Fig. 3). Concentrations and diameters of vapor bubbles in different layers of the metal differ from

each other (Fig. 4); they depend on the strain rate of tension in the rarefaction wave and on the metal temperature in the layer. When the volume fraction of vapor exceeds the volume fraction of the liquid phase, the consolidation of bubbles begins in the layer; the liquid phase is destructed on the drops (Fig. 5). Gradually the liquid phase fracture takes place in all area, in which the bubbles were generated by the tension. Further evolution of the two-phase medium is reduced to the expansion of droplets accompanied by the droplets coalescence due to the Brownian motion.

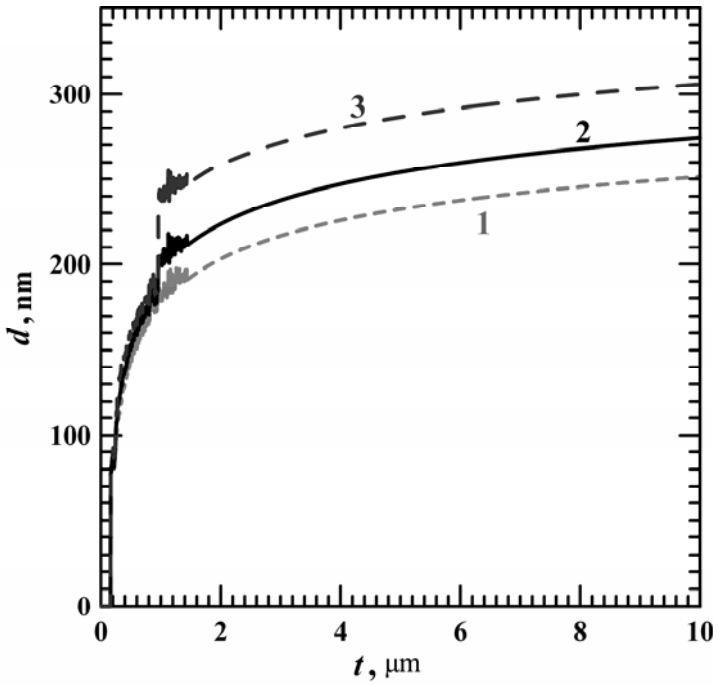

Figure 5. Time evolution of the average diameters of the drops: 1 – average on the number of drops, 2 – average on the drops surface areas, and 3 – average on the mass of the drops. The first drops are formed approximately 200 ns after the irradiation beginning in the layer with the maximal concentration of the vapor bubbles. A sharp increase of the average diameters is observed during the first 1 μs, it is connected with the gradual fracture of the liquid layers with lower concentration and, consequently, with the higher diameters of the vapor bubbles.

3. Conclusions

The mathematical model is proposed and the numerical investigation is performed of the metal fracture and fragmentation in the energy-release zone under the action of the high-current electron beam. The beam heats the metal and converts it in the metastable liquid state, which is destructed under the action of rarefaction wave propagating from the free (irradiated) surface of the metal. The tensile stresses of the value of about 2.5 GPa initiate the generation and growth of vapor bubbles. The following merging of the bubbles results in fragmentation of the simply connected liquid phase on the drops. Under the investigated conditions, the formation of the vapor bubbles begins 30 ns after the end of irradiation pulse. Concentration of the bubbles depends on the metal temperature and on the strain rate of tension in the rarefaction wave. This concentration determines the diameter of the resulting liquid drops, which varies from several tens up to several hundreds of nanometers in different parts of the energy release zone. Existence of the metastable state of expanded liquid results in propagation of the rarefaction wave with negative pressure of the value up to 2.5 GPa behind the shock wave in the deeper solid layers of the irradiated metal, which can substantially influence on the spallation of back surface in solid state as well.

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