Numerical study of mass transfer of a material under intense flows of high-speed electrons and plasma

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Abstract. The paper presents the mechanisms of mass transfer in a material under compressive plasma flows. The work contains numerical studies on mass loss from the surface of a sample treated by Compressive Plasma Flow, in the first case, and by High-Current Electron Beam, in the second case. The mass ablated from the material surface was computed with BETAIN software. The effects of plasma flow pressure on mass transfer of the material and processes of formation of the molten layer and erosion of mass from the material surface were investigated. It was revealed that plasma flow pressure formed a shock-compressed layer on the sample, and molten liquid was displaced from the center to peripheral regions. If sample size is less than the diameter of plasma spot, the melt is displaced out of the sample. This approach can explain experimental values of molten thickness and mass loss.

1. Introduction

Nowadays, the treatment of materials with intense energy flows (ion beams, low-energy high-current electron beams or compressive plasma flows) used to modify properties of a material is one of the promising methods in modification of structural materials [1]. This processing increases mechanical strength, microhardness, wear-resistance. The significant factor of the change of forming material properties is mass transfer occurring in the treated material.

Mass transfer in metal samples under low-energy high-current electron beams (LEHCEB) is well studied experimentally and theoretically in [1-4]. As shown in [4], the main mass transfer mechanisms under (LEHCEB) irradiation are thermodiffusion, Richtmyer–Meshkov instability (RMI) [5, 6], and thermocapillary convection [4, 7, 8].

A simple estimation of the role of thermodiffusion shows that over the metal melt lifetime (several tens of microseconds), the diffusion layer depth does not exceed 1 μm, which is much smaller than the mixing depth (10–20 μm) detected experimentally [2, 3]. Thus, the mass transfer by thermodiffusion takes place in material under intense energy flows, but this is not the main mass transfer mechanism.

Refs. [4, 7, 8] studied mechanisms of mass transfer during LEHCEB irradiation. It was shown that the main mechanism of mass transfer under LEHCEB treatment is thermocapillary convection.

Main mechanisms of mass transfer in material under LEHCEB irradiation were revealed, while in the case of processing by CPF, the results of numerical simulation strongly differ from experimental data. The paper considers the following mechanisms of mass transfer: thermodiffusion, thermocapillary convection and influence of plasma flow pressure on mass transfer.
The purpose of this work is to determine the influence of convection on mass transfer under CPF processing and to perform numerical study of the mass loss from the surface of a sample treated by LEHCEB and CPF.

2. Numerical results

Let us consider the role of convection in mass transfer of material exposed to CPF. The surface layers melt under CPF with the following parameters: discharge duration was about 100 µs, plasma flow velocity was (1-3)×10^4 m/s, plasma pressure on surface was up to 15 MPa [9, 10], and molten depth was up to 10-20 µm [11].

When a target is nonuniformly heated in its depth, a convective flow can appear. The following two types of convection are possible in a conducting material: thermocapillary convection and thermogravitational convection (which is caused by the acceleration of an irradiated medium). As shown in ref. [4], under heating metal target by LEHCEB, thermocapillary convection develops, while the role of thermogravitational one is negligible.

Thermocapillary convection can develop, when there is temperature gradient directing into target from free surface. Energy release of CPF is surface source, unlike the case of the energy release of LEHCEB. Therefore, the temperature gradient pointing in opposite direction, to the free surface, has stabilizing effect on volume flow. Temperature perturbations on an irradiated surface are always present, even at an ideally uniform beam current density, because of the surface microrelief. This can result in increased volume flow in the surface layer, namely, thermocapillary convection.

Let us consider the melt with the depth of 30 µm in 2D Cartesian coordinate system and temperature of T = 2200 K (which corresponds to experimental data) to study the role of thermocapillary convection. Non-uniform surface heating is simulated by heating of the round area of 2 µm in the center of the calculated domain with CPF heat flux (Fig. 1). Let us use the domain of 30x30 µm. On the boundary of melt-solid there is non-slip condition. On the one hand, the heat flux goes into inner layers of target due to heat conduction. On the other hand, surface layer gets heat from plasma flow. As surface tension is a temperature function, thermocapillary force arises. It directs from hotter zone to colder one.

Numerical simulation was conducted using the model presented in [4]. Fig. 2 presents results of the numerical research of temperature field at 50 µs without and with thermocapillary force. As shown in the figure, thermocapillary force induces formation of two vortexes which mix material efficiently.
and, as a result, temperature field becomes more uniform and temperature gradient directing to free surface decreases. Thus, non-uniform surface heating of the target excites volume flow that causes more uniform temperature volume distribution.

Figure 2. The results of the numerical research of temperature field at 50 µs without thermocapillary force (left) and with it (right).

The numerical calculation of melt depth and mass loss dependencies on absorbed energy density was run out by BETAIN software [12]. CPF processing was taken into account as heat flux on the free surface. Fig. 3 demonstrates the results of the numerical research of dependence of mass loss on absorbed energy density under CPF processing and LEHCEB irradiation.

Figure 3. The results of the numerical research of dependence of mass loss on absorbed energy density under CPF processing and LEHCEB irradiation.

The melt depth determined experimentally during LEHCEB with absorbed energy density of $W = 20 \text{ J/cm}^2$ was up to 20 µm, while the melt thickness specified by conductivity did not exceed 5 µm. Consideration of thermocapillary convection results in the decrease of melt thickness. Thus, due to thermocapillary convection, the surface molten layers have more uniform temperature, despite the increase of temperature gradient on the melt-solid boundary. Such gradient is less than heat flux on the free surface by CPF. And as a result, there is an intense ablation of thicker molten layer.
Such difference of experimental data from numerical results can be explained by the fact that the influence of shock compressed layer on material dynamics is not considered in the simulation of CPF processing. Taking the above mentioned into account, let us suppose that the target layer melts under CPF processing, then molten liquid displaces from the area of high plasma pressure to peripheral regions due to the influence of shock-compressed layer on material. If sample size is less than the diameter of plasma spot, the melt is displaced out of the sample.

Mass displacement tends to outcrop deeper material layer exposed to CPF. Such dynamics of material heating ensures deeper melting of target than that due to heat conductivity. Surface tension levels the melt until material crystallization after CPF treatment end.

The numerical study of the influence of shock-compressed layer on melt dynamic was carried out to confirm proposed mechanism of relief formation depicted in Fig. 4. For this purpose, the model [13] of potential flow of incompressible liquid in 2D Cartesian coordinate system has been applied. Molten volume was simulated by half-infinite media with plane surface. Mass density, surface tension and coefficient of viscosity were taken from [14] at temperature of 1800 K. Linear dimensions correspond to experimental data which results are shown in Fig. 5. Numerical calculation was performed for 200 µs which is about the life time of melt, while shock-compressed layer was taken into account during CPF processing, namely during 80 µs.

![Figure 4. The sample surface exposed to CPF with the deposed film [15].](image1)

![Figure 5. The numerical sample surface profile after CPF processing.](image2)

The calculation shows capillary waves developing on the sample surface under CPF processing, while after CPF processing end, there is perturbation amplitude growth due to Richtmyer–Meshkov instability until crystallization.

Fig. 5. represents numerical sample surface profile after CPF processing. As figure shows wave-like relief forms at CPF processing. A breastwork arises due to plasma pressure forming shock-compressed layer that is observed experimentally. The numerical research has revealed that breastwork width depends on pressure and linear dimensions of the region, which is subjected to action of shock-compressed layer. Calculated amplitude of perturbation under crystallization depending on conditions (plasma flow pressure, melt lifetime) is from 10 to 40 µm, which is in accordance with experimental melt thickness.

3. Conclusion
In the paper, the numerical research on mass loss from target surface under treatment by compressive plasma flows and high current electron beam has been conducted.
It was numerically shown that non-uniform heating of target surface results in the development of volume flow, which made temperature more uniform in molten volume.

It was revealed that plasma flow pressure-formed shock-compressed layer on sample and molten liquid is displaced from center to peripheral regions. If sample size is less than the diameter of plasma spot, the melt is displaced out of the sample. This approach can explain experimental values of molten thickness and mass loss.

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