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Model of convection mass transfer in titanium alloy at low energy high current electron beam action

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Abstract. The convection mixing model is proposed for low-energy high-current electron beam treatment of titanium alloys, pre-processed by heterogeneous plasma flows generated via explosion of carbon tape and powder TiB_2. The model is based on the assumption vortices in the molten layer are formed due to the treatment by concentrated energy flows. These vortices evolve as the result of thermocapillary convection, arising because of the temperature gradient. The calculation of temperature gradient and penetration depth required solution of the heat problem with taking into account the surface evaporation. However, instead of the direct heat source the boundary conditions in phase transitions were changed in the thermal conductivity equation, assuming the evaporated material takes part in the heat exchange. The data on the penetration depth and temperature distribution are used for the thermocapillary model. The thermocapillary model embraces Navier-Stocks and convection heat transfer equations, as well as the boundary conditions with the outflow of evaporated material included. The solution of these equations by finite elements methods pointed at formation of a multi-vortices structure when electron-beam treatment and its expansion over new zones of material. As the result, strengthening particles are found at the depth exceeding manifold their penetration depth in terms of the diffusion mechanism.

1. Introduction

Titanium alloys are widely applied in various industries, e.g. in aircraft engines construction for manufacturing blades and discs. The thickness of damaged layers varies 10 to 20 μm as seen in the process of gas-turbine engines maintenance [1]. Therefore, it is necessary to develop technologies of surface modifying titanium alloys. At present a great variety of ways and methods of surface modification are developed, inter alia, the treatment by low energy high current electron beams [2]. This kind of treatment is advantageous as its pulse-periodic character allows of keeping surface layers in the molten state for a longer period of time, and it provides the effect of hardening, which furthers formation of submicro- and nanostructures [3]. The shortcoming of electron beam treatment is forming craters on the surface of materials [4], which are dangerous stress risers when cyclic stressing. Thus, treatment conditions with minimal influence of craters are to be selected; moreover, the thickness of the layer to be modified should not exceed it of the layer damaged in the process of maintenance. The information how electron beam treatment influences materials is necessary in order to search for the modes mentioned above. As shown in [4 – 10] electron beams have a multifactorial effect on

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materials. It comprises heating, melting and evaporation of materials from the surface. When melting metals electron beams might cause formation of closed streams in the melt. The intensity and character of these streams are relevant for heat and substance transfer, which, in their turn, influences diverse technological processes. These streams might be formed and developed due to thermocapillary forces [8 –10]. The phenomenon of thermocapillary convection has been studied in various works. A double-vortices stream is formed for the definite, quite high Marangoni numbers [10]. The mathematical model of heat and mass transfer in the target irradiated by intense beam of charged particles was proposed in [8, 9], it involves equations of continuum mechanics, kinetic equation for fast particles and is enclosed by the wide-range equations of state. The basic mechanism of liquid phase heat and mass transfer is revealed to be thermocapillary convection and instability according to the results of calculations [9]. Moreover, it is possible when pulse duration is far shorter than the typical period of thermal diffusivity. Two oppositely directed vortices are formed in the sub-surface layer. The big vortex is the result of the surface tension force which depends on the temperature; whereas the small vortex arises as the inflow of liquid involved by big vortex exceeds the outflow, causing the formation of the dead zone and small vortex, as the consequence [8, 9]. However, evaporation from the material surface has not been taken into consideration in these works, although the high power density of the beam q ~ 10^6 – 10^9 W/cm^2 leads to heating up the metal surface, as the result, it starts melting and evaporating together with the forming plasma flame [5]. The thermal conductivity equations and the gas-dynamic problem of gas dispersion are to be solved to calculate the temperature distribution. The evaporation is irrelevant for power density q ≤ 10^6 W/cm^2, so the power density of a heat flow is required for solution of the heat problem [5]. Otherwise, extraordinary high temperatures might be the result of the direct heat flow on the boundary [6]. Therefore, the authors [6] suggest the enthalpy statement of the problem with changing boundary conditions, which can register phase transformations automatically. The penetration depth increases linearly with the going up power density of electron beam according to the calculations, the pulse duration has principally no influence on it. In case electron beams influence the material exposed to heterogeneous conductor electric explosive-produced plasma flows, it is more difficult as heat, generated in the process of forming and dissolving phases, is to be considered. The effects of electron beam on titanium pre-processed by heterogeneous graphitize carbon fibers explosive-produced plasma flow is studied in [8]. The electron beam is found out to be the reason for dissolution of carbon particles, moreover, the period of dissolution depends on the radius of a particle. Therefore, we can conclude a mathematical model describing convection mixing, which involves phase transitions in conditions of electron beam treatment, is currently not available, and our work is aimed at the development of such a model.

2. Mathematical model

Let us consider the effect of electron beams on the plate (Figure 1). The input parameters of the problem are as follows: E_s – surficial power density, t_0 – pulse duration and radius of the impact – R_0 .

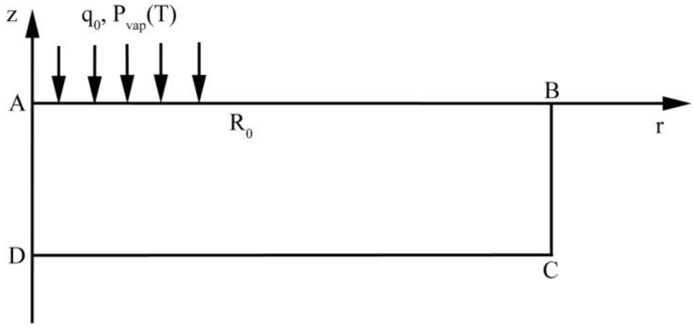


Figure 1. Computational domain scheme

The equation of thermal conductivity is written.

$$\rho \tilde{N}_p \frac{\partial T}{\partial t} = \nabla \cdot \left(k \nabla T \right) \quad (1)$$

As we focus on the distribution of temperature over the depth of the sample we consider the one-dimensional case only. We model phase transitions on the boundary via setting the temperature-dependent characteristics of material:

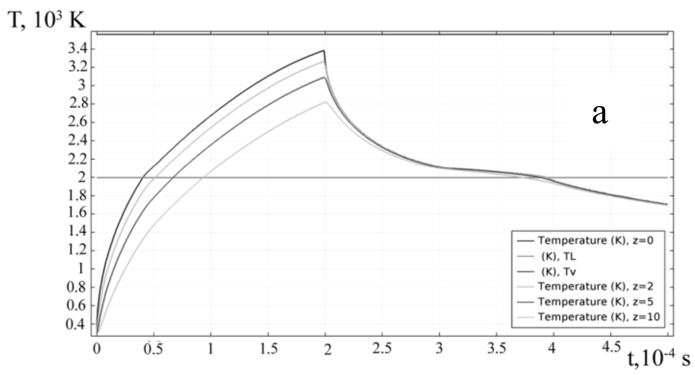
$$\tilde{N}_p(T)\rho(T) = \begin{cases} C_S \rho_S, T < T_L \\ \dfrac{L_L \rho_L}{\Delta T_L}, T_L \le T < T_L + \Delta T_L \\ C_L \rho_L, T_L + \Delta T_L \le T < T_V \\ \dfrac{L_V \rho_V}{\Delta T_V}, T_V \le T < T_V + \Delta T_V \\ C_V \rho_V, T_V + \Delta T_V \le T \end{cases}, \quad k(T) = \begin{cases} k_S, T < T_L \\ k_S + \dfrac{(k_L - k_S)(T - T_L)}{\Delta T_L}, T_L \le T < T_L + \Delta T_L \\ k_L, T_L + \Delta T_L \le T < T_V \\ k_S + \dfrac{(k_V - k_L)(T - T_V)}{\Delta T_V}, T_V \le T < T_V + \Delta T_V \\ k_V, T_V + \Delta T_V \le T \end{cases} \quad (2)$$

Heat losses caused by evaporating material were not taken into account in boundary conditions [7], therefore, the coefficient of thermal conductivity was selected in order to describe experimental data. We take these losses into consideration and use the model proposed in [12]. The conditions on the boundary AB with phase transitions taken into account are written in the form:

$$-\vec{n} \cdot \vec{q} = q_0(t) - q_{out}(T) = \frac{E_s}{t_0} \theta(t) - \dot{m}(T) L_V \quad (3)$$

Where $\dot{m}(T) = (1-\beta)\sqrt{\dfrac{M}{2\pi RT}}\, p_0 \exp\left(\dfrac{L_V M (T - T_V)}{RTT_V} \right) -$ mass flow through the boundary.

When the substrate evaporates the residual gas in the chamber takes part in the heat exchange. Some energy dissipates; the other part goes back to the substrate keeping it at the vaporization temperature longer than the period of impact. We assume heat capacity of the evaporated phase C_V =20 MJ kg^{-1} K^{-1} for numerical modelling of this gaseous layer. It allows of making a 1-2 μm thick heat “buffer”, which will keep the putting in power and emit it gradually. Hence, setting the heat capacity of the gaseous phase we can model the boundary conditions [7], considering, however, heat losses caused by gaseous phase dissipation. It makes it possible to develop a more complete model of heat processes arising in the process of electron beam treatment, which describes experimental data on the penetration depth. The distribution of temperatures in titanium at various penetration depths and in diverse modes of irradiation is presented in Figure 2. As one can see the temperature on the surface does not reach the evaporation temperature at E_s = 45 J/cm^2, t_0 = 200 μs, and it drops in the point t_0 (Figure 2a). In conditions E_s = 65 J/cm^2, t_0 = 100 μs the temperature on the surface comes up to the evaporation temperature and is constant for the period 180 μs (Figure 2b), then it falls sharply.



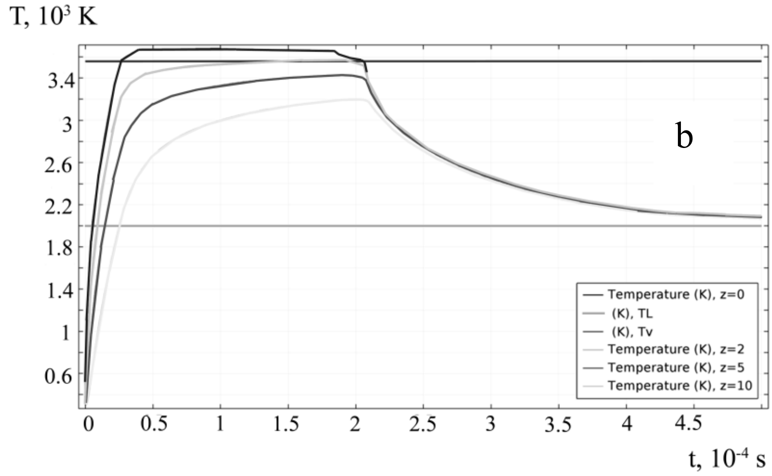


Figure 2. The distribution of temperature in titanium in the process of electron beam treatment
a) E_s = 45 J/cm^2, t_0 = 200 µs; b) E_s = 65 J/cm^2, t_0 = 100 µs

Therefore, the heat "buffer" made by the evaporated material leads to stabilization of the temperature on the surface and over the depth of the sample for the period exceeding the pulse duration. As the result, the gradient of the undisturbed temperature throughout the depth is constant, developing the conditions for the thermocapillary instability. The initiation of this instability is analyzed in metals and binary alloys in the process of electron beam treatment [13], the dispersion equation is obtained too. On the base of this equation the critical wavelength with the maximum of the disturbance decrement was determined. Its value approximates to 100 nm. The crystallization cells are of the same range. Developing the numerical model of the thermocapillary convection we take into consideration the change in the surface curvature. We solve the axis-symmetrical problem for Navier Stocks equation and heat transfer to model the convection flows. The conditions on the boundary AB (Figure 1) are in the form:

$$\begin{aligned} -\vec{n}\cdot\vec{q} &= q_0(r,t) - q_{out}(T) = \frac{E_s}{t_0}\exp\left(-\frac{r^2}{R_0^2}\right)\theta(t) - \dot{m}(T)L_V \\ p &= p_0 + p_V,\, p_V = \frac{1+\beta}{2}(p_c - p_0) \end{aligned} \tag{4}$$

where p_V – pressure of vapor output, p_c – Clapeyron pressure. On boundaries BC, DC: $\vec{n}\cdot\vec{q} = 0, \vec{n}\cdot\vec{\mathrm{v}} = 0.$ The problem was solved by the finite elements method in the software Comsol Multiphysics. To model the free surface we used the moving mesh method. The input parameters of the problem are given in Table 1.

Table 1. Material properties of the sample.

Symbol	Nomenclature	Value
ρ_S	Solid density	4500 kg m^{-3}
ρ_L	Liquid density	4100 kg m^{-3}
ρ_V	Vapor density	4100 kg m^{-3}
C_L	Liquid heat capacity	922 J kg^{-1} K^{-1}
C_S	Solid heat capacity	630 J kg^{-1} K^{-1}
C_V	Vapor heat capacity	$2\cdot10^7$ J kg^{-1} K^{-1}
k_L	Liquid thermal conductivity	30 W m^{-1} K^{-1}

k_S	Solid thermal conductivity	25 W m^{-1} K^{-1}
k_V	Vapor thermal conductivity	30 W m^{-1} K^{-1}
μ	Coefficient of dynamic viscosity	0.0021 kgm^{-1} s^{-1}
L_L	Melting latent heat	304 kJ kg^{-1}
L_V	Vaporization latent heat	8900 kJ kg^{-1}
σ_0	Surface tension coefficient	1.872 N m^{-1}
$d\sigma / dT$	Thermal gradient of surface tension	$-49\cdot10^{-5}$ N m$^{-1}\cdot$K^{-1}
E_s	Pulse energy	450 kJ m^{-2}
r_0	Radius of the impact	200 μm
M	Molar mass	0.047867 kg mol^{-1}
T_L	Melting temperature	1998 K
T_V	Vaporization temperature	3650 K

The results of calculations are given in Figure 3

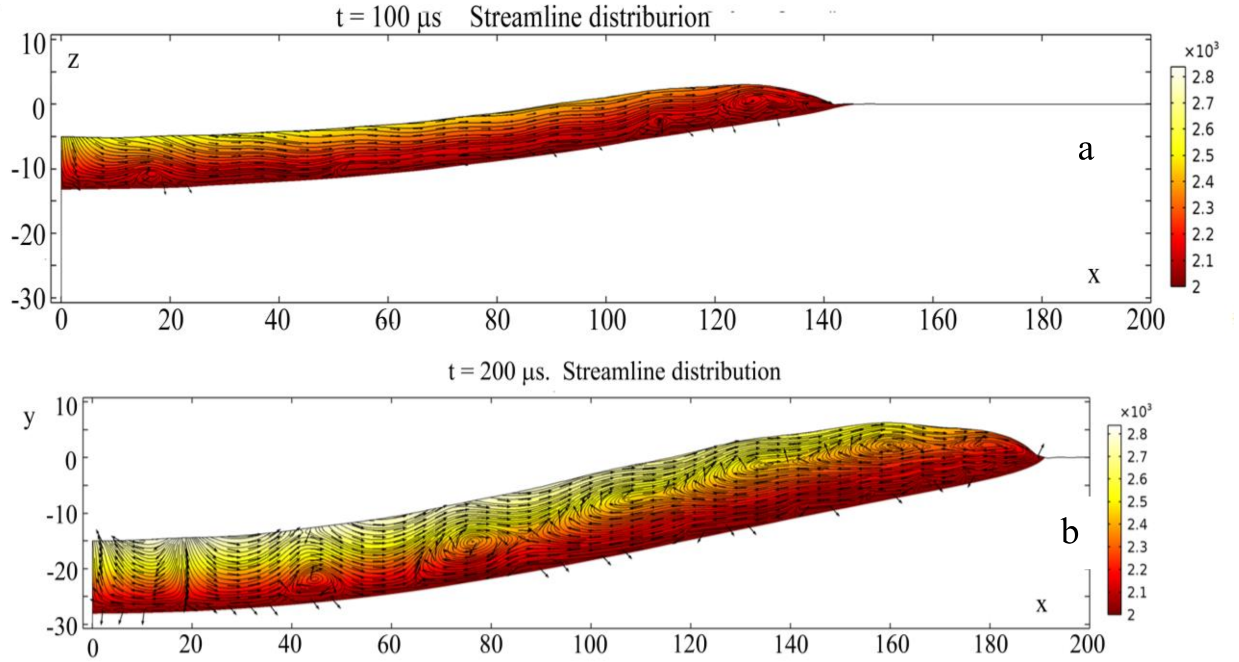


Figure 3. The distribution of streamlines at various time points
a) t =100 µs; b) t = 200 µs

The convection of material in the molten layer as well as its probable effect on heat transfer and geometry of the pool were not taken into consideration in all the works focused on electron beam melting, except [14]. The latest works on EBM modelling [15, 16] revealed it was not possible to obtain multi-vortices flow in the melt layer. In our calculations we have obtained parameters of the multi-vortices flow (Figure 4). This fact is principally important for mixing the melt and creating homogenous distribution of boron-containing particles, which is necessary for determining the mechanism of wear resistance improvement [11]. The distribution of microhardness over the depth and the thickness of the strengthening zone, calculated on its base, confirm, the proposed model of convection mass transfer can provide an adequate description of the processes when electron-beam treatment [11].

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