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SIMULATION OF THERMOPHYSICAL PROCESSES OCCURRING IN TRANSITION OF THE SURFACE METAL LAYER OF A MOVING STRONG-CURRENT GAS DISCHARGE ELECTRODE TO AN AMORPHOUS STATE

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We carried out a numerical simulation of the melting and solidification of a surface layer for various metals and heating parameters with account for phase transitions. We determined the conditions enabling the formation of amorphous metallic structures. The conditions were shown to be realized when the heat source was a steady-state strong-current gas-discharge plasma.

The specific feature of interparticle interactions and, correspondingly, of the physical, chemical, and mechanical properties of amorphous metallic materials lies in the absence of long-range order in the arrangement of microcrystalline structural units (atoms, ions, molecules), which is typical of a crystalline state. The solid amorphous phase corresponds to the limiting state of a metastable solid body and can be obtained by various means: solidification from a melt, chemical precipitation from a solution or electrolyte, irradiation of a crystalline material by concentrated energy fluxes, etc. [1, 2]. In practice, the technique of a rapid chilling of a liquid phase is used for the production of metallic glasses.

According to the cluster model, the viscosity of metal melts increases substantially on supercooling. As a result, at sufficient rates of cooling and solidification a cluster structure is investigated in the solid state, and an amorphous phase is formed on its basis. As the rate of melt cooling W_0 decreases, a partially or fully microcrystalline structure is formed with a characteristic disorientation of crystallites with respect to one another.

A high rate of cooling can be attained by the fast removal of thermal energy from the bulk of the melt. One of the promising methods is the short-duration exposure of a metal article to concentrated energy fluxes (laser beam, electron beam, plasma flux). This results in strong local heating of the surface layer, its melting, and subsequent rapid chilling of the melt due to thermal contact with the remaining mass of the article (hardening by its own substrate).

In [3-6] the possibility was considered of using for this purpose pulsed plasma injectors with a heat flux density of up to 10^9 W/cm^2. Stationary plasma generators are preferable in practice. Compared with pulse generators, they are more simple and provide high reliability and the possibility of using reliable methods to control technological processes. According to [7, 8], electric-arc plasma generators ensure the production of continuous high heat fluxes $q > 10^4$ W/cm^2, which, in a primary consideration, can lead to a substantial modification of the surface layer of metals.

In the present work we consider the possibility of using a PS-1V atmospheric-pressure electric-arc apparatus [9] to bring metals to an amorphous state. The article under investigation, namely a plasmotron anode, is made of various materials (copper, iron, zinc, etc.). The velocity of the anode surface perpendicularly to the discharge axis is regulated within the range of 0.5–10 m/sec. The diameter of the zone of material exposure to the arc is 1–2 mm; consequently, the characteristic time of the thermal effect is $t_{\text{ef}} = 0.1-4$ msec. The density of the heat flux to the anode surface is 10^3-10^6 W/cm^2. The uniformity of the distribution of q over the heating spot

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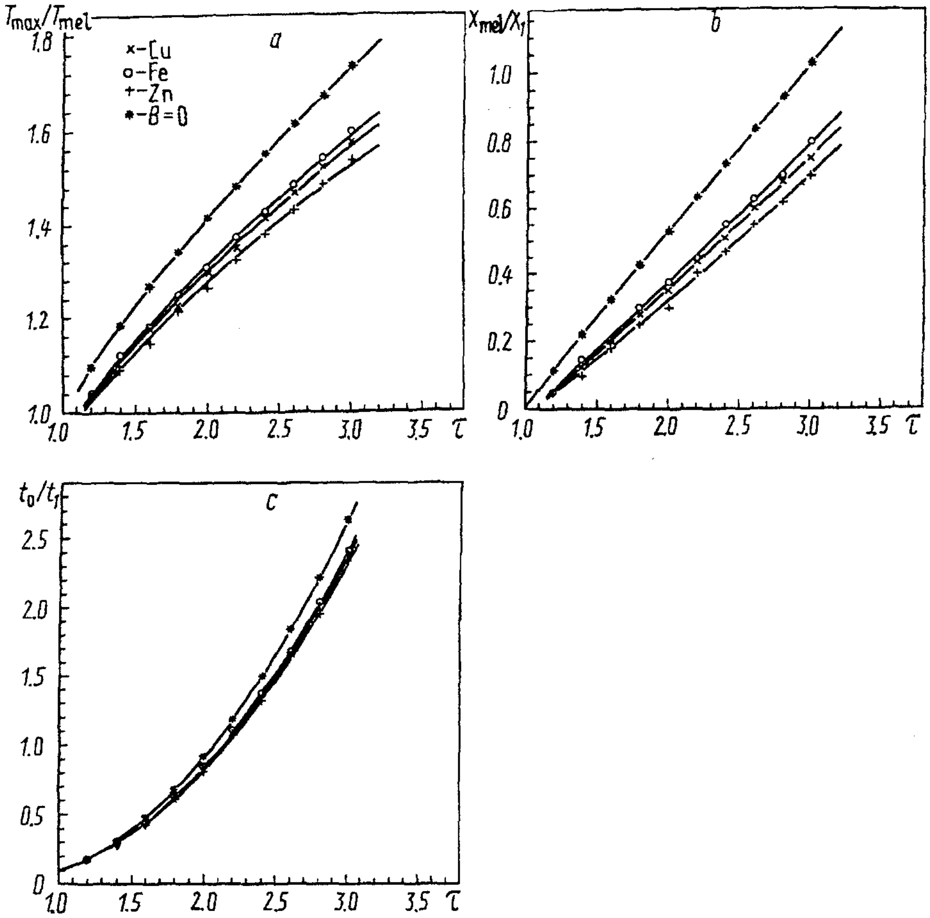

Fig. 1. Maximum surface temperature (a), depth of melting (b), and time of cooling of the surfaces of various metals from T_{max} to $0.75T_{mel}$ (c) versus the duration of the thermal effect (in dimesnionless units).

can be attained by selecting discharge conditions under which diffuse attachment of the arc to the anode is observed [8, 9]. In this case the exposure time of a fixed zone of the anode to the arc is decreased, as are the amount of erosion and local distortions of the electrode surface. Investigations have shown that the described apparatus rather uniformly melts the surface layer of a cylindrical anode.

The thickness of the melted layer and the magnitude of the needed energy density are the principal parameters for selecting the means of heating a surface to bring the layer to an amorphous state; they can be determined from the well-known thermophysical properties of the material and the duration of the thermal effect. For this purpose, we carried out a numerical simulation of a thermophysical process.

We considered the process of melting and solidification of a semi-infinite metal plate exposed to a heat source of constant power which is fully absorbed by the surface. The heat conduction equation is solved for the region near the center of a heating spot of radius r, at which the condition $r \gg (at_{ef})^{1/2}$ is satisfied. This case allows a one-dimensional consideration of the problem. The thermophysical characteristics of the metal and its melt are considered to be identical and independent of temperature; they are taken from [11]. According to estimates, the error of this approximation for Zn, Ti, Ni, and Cu over the time and space coordinates does not exceed 10 and 25%, respectively.

After heating of the plate surface up to the melting temperature, a melted layer is formed, and the interface between the solid and liquid phases begins to move lower into the target. Here, the latent heat of melting L is absorbed. On termination of thermal effect, the surface cools off, and the temperature equalizes over the depth of the plate. Phase-transition heat evolves at the solidification front. The phase transition heat should be smaller than L, since it is assumed that a crystalline lattice is not formed. According to [12], it is taken to be equal to $0.5L$ for pure metals.

TABLE 1. Error (%) for $T_{\max}$, X_{mel}, and t_0 Introduced by the Neglect of Phase Transitions

τ_{ef}	$\Delta T_{\max}/T_{\max}$		$\Delta X_{\text{mel}}/X_{\text{mel}}$		$\Delta t_0/t_0$	
	$B=0.3$	$B=0.5$	$B=0.3$	$B=0.5$	$B=0.3$	$B=0.5$
1.4	5	9	50	110	7	–
2.0	8	12	40	75	9	13
2.4	8	12	30	55	9	13

There are several approaches to the solution of such a problem. In [13], an approximate analytical method is suggested that employs phenomenological notions about the form of the melting depth function. In [14], to find the discontinuity at the interface between the liquid and solid phases it is assumed that materials are melted in a small but finite temperature range, rather than at a certain temperature. This reduces the problem of melting to the problem of the thermal conductivity of a phase with temperature-depending properties. The latent heat of melting manifests itself as an increase in the specific heat near T_{mel}:

$$\frac{\partial H}{\partial T} = \rho \left(c + L \frac{\partial s}{\partial T} \right).$$

To find the solution in conformity with the algorithm suggested, it is also necessary to make assumptions about the character of melting.

Let us introduce the dimensionless quantities: $\tau = t/t_1$, $\chi = x/X_1$, $B = L/cT_{\text{mel}}$, $\theta = (T - T_0)/T_{\text{mel}}$, $h = H/\rho c T_{\text{mel}}$, where $t_1 = \pi \lambda c \rho (T_{\text{mel}}/2q)^2$ is the time of the start of melting, and $X_1 = (a t_1)^{1/2}$, and let us formulate a heat-conduction problem for the heat function, which will be written as $H = \rho(cT + \varepsilon L)$. To take phase transitions into account, we introduce here the parameter ε, which is volumetric fraction of the melt.

After the attainment of $T = T_{\text{mel}}$, the value of ε begins to vary from 0 to 1 for the time necessary for the latent heat of phase transition to be absorbed. Since it is assumed that solidification occurs without the formation of a crystalline lattice, then after the attainment of $T = T_{\text{mel}}$ in solidification the value of ε changes from 1 to 1/2 for the time needed for the solidification heat $L/2$ to evolve.

The problem is formulated as follows:

$$\frac{\partial h}{\partial \tau} = \frac{\partial^2 \theta}{\partial \chi^2}; \quad \chi \ge 0, \qquad \left.\frac{\partial \theta}{\partial \chi}\right|_{\chi=0} = -(\pi)^{-1/2}/2; \quad 0 \le \tau \le \tau_{\text{ef}}. \tag{1}$$

As the initial conditions, we select the temperature distribution obtained from an exact analytical solution of the heat conduction equation at the time moment $t = t_1$:

$$\theta(\chi, 1) = (\pi)^{1/2} \operatorname{ierfc}(\chi/2). \tag{2}$$

The spatial drivatives in (1) are replaced by finite-difference analogs:

$$\frac{\partial^2 \theta}{\partial \chi^2} \approx \frac{\theta_{n-1} - 2\theta_n + \theta_{n+1}}{(\Delta\chi)^2}, \qquad \left.\frac{\partial \theta}{\partial \chi}\right|_{\chi=0} \approx \frac{\theta_2 - \theta_0}{2\Delta\chi} = q^*, \quad q^* = -\frac{(\pi)^{-1/2}}{2}.$$

The resulting system of ordinary differential equations with the right sides

$$F_1 = 2/(\Delta\chi)^2 (\theta_2 - \theta_1 - \Delta\chi\, q^*);$$

$$F_2 = 1/(\Delta\chi)^2 (\theta_{i-1} - 2\theta_i + \theta_{i+1}), \quad i = 2, \ldots, N-1;$$

$$F_N = 0$$

TABLE 2. Parameters of Thermal Processes at which the Formation of Amorphous Metallic Structures is Possible ($q = 10^5$ W/cm^2, $W_0 = (T_{max} - 0.75T_{mel})/t_0$)

Metal	t_{ef}, msec	X_{mel}, μm	W_0, 10^6 K/sec
Zn	0.1–0.25	4–40	10–2.5
Ti	0.2–0.5	5–30	20–4
Fe	0.4–0.8	8–35	7–2.5
Ni	0.8–1.8	10–80	4–1
Cu	2–2.5	20–70	1.3–0.8

is solved by a numerical method.

The time and space intervals and the remaining computation parameters were selected, for practical considerations, for coincidence with third-place accuracy of the numerical solution of the problem with zero initial conditions and exact analytical solution (2).

For the range $\tau_{ef} = 1-3$ we calculated the maximum temperature of surface, the depth of melting, and the time of the surface cooling from T_{max} to $T = 0.75T_{mek}$ (Fig. 1). The value $T = 0.75T_{mel}$ corresponds to a deep supercooling of the melt, which is a condition for the homogeneous incipience of an amorphous phase [2, 3]. The calculation was performed for various metals and for the case when the latent heat of phase transitions is ignored ($B = 0$).

For the majority of metals, the characteristic of the phase transition B varies from ~ 0.3 ($B_{Ti} = 0.3196$) to ~ 0.5 ($B_{Zn} = 0.5127$). The error that can be introduced by ignoring phase transitions depends on the value of B and on the duration of the heat pulse (see Table 1). From the table it is seen that ignoring the latent heat of phase transitions can introduce a substantial error when determining the depth of melting, without giving large distortions in the field of temperatures.

Table 2 shows that in order to realize rates of melt cooling $W_0 \sim 10^7-10^6$ K/sec, it is necessary to have heat fluxes on the order of 10^5 W/cm^2. For smaller q it is impossible to attain high rates of cooling, since $W_0 \sim q^2$. But since the duration of the thermal effect is limited by the time of heating of the surface to the boiling temperature ($\sim 1/q^2$), an increase in q leads to a decrease in the possible depth of melting ($X_{mel} \sim 1/q$). Therefore, to obtain a layer of supercooled melt of required thickness, it is necessary to carry out optimization using the value of q.

Analysis of predicted data and technological possibilities of the proposed apparatus shows that by using steady-state plasma flows generated in the anode region of high-current gas discharges it is possible to obtain amorphous structures on the surfaces of metallic cylindrical articles.

NOTATION

W_0, rate of cooling; q, heat flux density; t_{ef}, time of thermal effect; a, thermal diffusivity of metal; t and x, time and space coordinates; T_{mel} and L, melting temperature and latent heat of the melting of metal; s, function of the depth of melting; H, thermal function (enthalpy); T, temperature; ρ, density; c, specific heat; τ, χ, B, θ, h, dimensionless quantities corresponding to t, x, L, T, H; ε, dimensionless parameter having the meaning of the volumetric fraction of the melt; T_{max}, maximum surface temperature; X_{mel}, depth of melting; t_0, time of surface cooling.

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