HEAT AND MASS TRANSFER IN THE SURFACE LAYER OF METALS UNDER LASER MACHINING

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The results are reported of computational and theoretical studies of the thermohydrodynamic processes in the surface layer of metals under the effect of single laser pulses.

1. It is of great practical importance to study heat and mass transfer in laser surface treatment and machining of metals. A need for a clear understanding of the distinctive features of heat and mass transfer under the effect of laser pulses of different energies and length arises during doping from the vapor and liquid phases, surface hardening, cutting and welding of metals by laser radiation, etc. Computational—theoretical modeling is important in research on the physics of processes that accompany laser machining and treatment of materials. We should point out that a number of urgent problems of laser technology can be investigated only on the basis of self-consistent physical models describing the heating, melting, and motion of melt under vapor outflow pressure and surface tension as well as radiation diffraction and dissipation of electromagnetic energy in the surface layer of the material. Earlier [1, 2] we proposed a numerical model, which gives a self-consistent description of the interrelated heat and mass transfer when linearly polarized laser radiation acts on a metal. On the basis of the developed model [1, 2] we study problems of importance for laser machining and thermochemical treatment, concerning the expulsion of melt by a single laser pulse according to an instability mechanism when a splash of melt is initiated by the development of small-scale perturbations on the surface of the metal and also pertaining to the stimulation of convection in the layer of melt.

2. Arutyunyan et al. showed [3, 4] that in the case when short pulses of radiation act on the surface and the focal spot is large the condition for melt to flow in the entire spot during the pulse is not satisfied and the splashing of melt should be affected substantially by small-scale nonuniformities in the vapor pressure on the surface of the metal. When the vapor pressure undergoes deep spatial modulation with a characteristic scale ~ Λ the velocity of the melt increases by a factor of r_f/Λ in comparison with the case when melt is expelled from the center of the laser beam toward the periphery; the velocity then is of the order of [3]

$$V = \int_0^\tau p\,dt/(\rho\Lambda). \tag{1}$$

When the condition [3]

$$V > \Lambda/\tau_m \tag{2}$$

is satisfied the velocity is sufficient to splash a considerable part of the melt. When melt is expelled as a result of deep spatial modulation of the vapor pressure, drops form with a characteristic size

$$r_0 \geqslant \sqrt{\chi\tau}, \tag{3}$$

which is substantially smaller than the drop size when the vapor pressure has a smooth profile

$$r_0 \approx (\pi r_f \sqrt{\chi\tau})^{1/3}. \tag{4}$$

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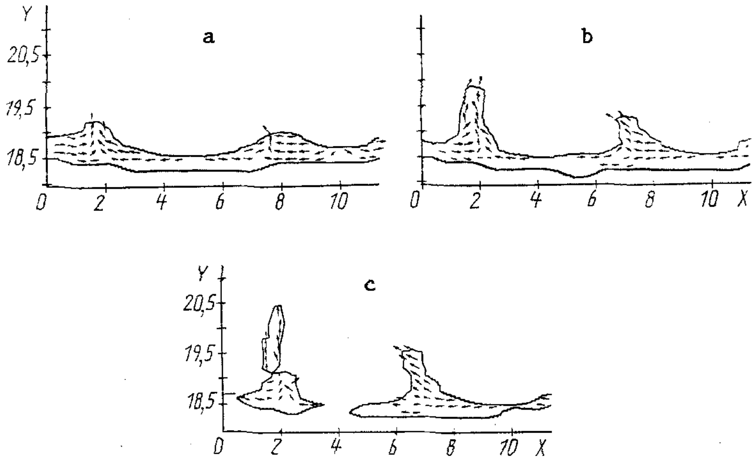

Fig. 1. Dynamics of the expulsion of melt by the instability mechanism under a square laser pulse of length 0.04 μsec and radiation intensity $5 \cdot 10^8$ W/cm^2, angle of beam incidence θ = 0.1: a) t = 0.041; b) 0.055; and c) 0.069 μsec. X, Y, μm.

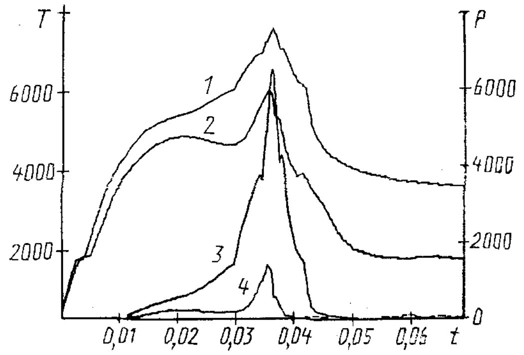

Fig. 2. Time dependence of the maximum and minimum temperature (curves 1, 2) and evaporative pressure (curves 3, 4); the radiation parameters are the same as in Fig. 1. T, K; P, atm; t, μsec.

The vapor-pressure modulation may be due to the initial small-scale structure of the laser beam and the development of light-induced surface structures on the surface of the melt. Splashing of melt under the effect of a laser beam with a spike structure was studied numerically earlier [3, 4]. At the same time, the important practical problem of a considerable part of the melt being splashed out as a result of the development of small-scale surface structures has not yet been explored in the literature.

The expulsion of melt by the instability mechanism was considered in the following formulation. We assumed that the focal spot size r_f substantially exceeds all of the characteristic spatial scales of the problem; accordingly, a wave incident on the surface of the metal can be assumed to be a plane wave. We considered the case when the radiation incident on the surface of the metal is polarized in a plane perpendicular to the plane of incidence (s polarization). The formation of a surface structure was described in the approximation of the interaction of three modes of relief. Gandel'man and Kondratenko [5] showed that at surface-structure amplitudes not greater than $h \lesssim (n/(n^2 + m^2))^{1/2}$ (here n and m are the real and imaginary parts of the dielectric constant of the medium), the closed system of interacting gratings includes the most rapidly growing Fourier component of the relief with period

$$\Lambda_1 = \lambda \Big/ \left(\cos^2 \theta + \left(\frac{n + m}{n^2 + m^2} \right)^2 \right)^{1/2}, \qquad (5)$$

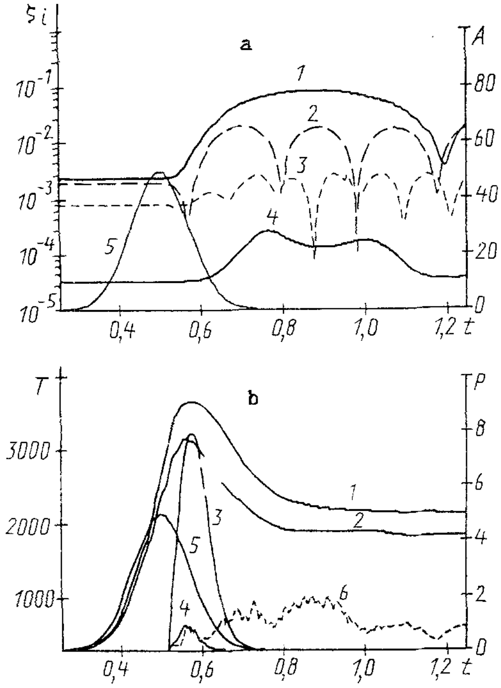

Fig. 3. Time dependence of: a) amplitudes of surface structures with periods Λ_1, Λ_2, and Λ_3 (curves 1-3) and uniform absorptivity (4) under the effect of a Gaussian radiation pulse (5) with a peak intensity of 10^8 W/cm^2; b) maximum and minimum surface temperatures (curves 1, 2), evaporative pressure (3, 4), maximum pressure of surface tension forces (σ) (5 is the shape of the laser pulse); angle of incidence $\theta = 0.5$ rad. ξ_i, μm; A, %.

as well as a grating with period $\Lambda_2 = \Lambda_1/2$; even though it has a smaller growth increment in the linear stage, the latter begins to compete with grating (5) at larger corrugation amplitudes. The grating with period $\Lambda_3 = \Lambda_1/3$ was introduced into the discussion to check the applicability of the approximation used. In accordance with the terminology adopted in the literature, the grating with period Λ_1 will be called a resonance grating and those with periods Λ_2 and Λ_3, supplementary gratings.

The diffraction of laser radiation on a surface structure consisting of superposition of three modes with periods Λ_1, Λ_2 and Λ_3 was studied in the Rayleigh approximation. The numerical algorithm for the computation of the diffracted fields and energy dissipated in the surface layer of the material was discussed in [2]. In all the cases under consideration the laser pulse length corresponded to the formation of comparatively deep structures with an amplitude not exceeding the limit of applicability of the Rayleigh method and the corrugation became deeper inertially until a drop formed. The problem of describing the absorption of electromagnetic radiation on a surface with a deep surface structure thus did not arise.

The temperature fields were calculated, the free boundary and the phase-transition boundary were determined, and the motion of melt under the effect of the pressure of vapor outflow and surface tension was simulated in accordance with the SOLA-VOF method, which was discussed in detail in [6].

The expulsion of melt by the instability mechanism was studied numerically on the example of the interaction of IR radiation with $\lambda = 10.6$ μm on the surface of iron, whose dielectric constant was assumed to be $\varepsilon = (10.1 + 14.6)^2$ [7]. The laser pulses were assigned a square or Gaussian shape. The pulse length was 0.01-0.5 μsec and the average radiation intensity in a pulse varied from $5 \cdot 10^7$ to 10^9 W/cm^2. As we see from Fig. 1, the resonance grating grows rapidly in the initial stage of formation of the surface structure; the amplitude of this grating substantially exceeds that of the positive Λ_2 and Λ_3. Later the surface structure with period Λ_2, whose amplitude becomes equal to that of grating Λ_1 by the end of the laser pulse, is the most rapidly growing Fourier component of the relief. For a time after the laser

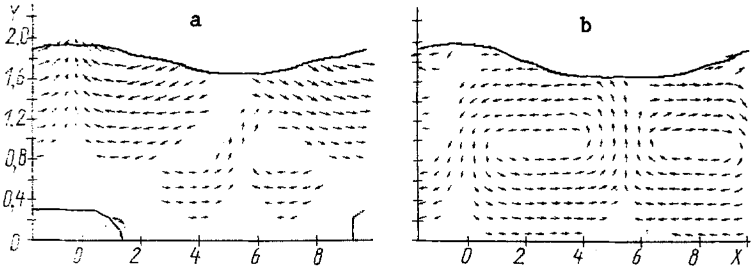

Fig. 4. Structure of flow in a film of melt: a) t = 0.775 μsec; b) 0.885 μsec; irradiation conditions as in Fig. 3.

pulse, nonuniformity persists in the heating of the surface and a rather high vapor pressure is maintained (Fig. 2). As a result the structure with period Λ_2 grows deeper and becomes dominant by the time $t \sim 0.05$ μsec. Melt is expelled inertially from the high-pressure region under the action of a pulse, conveyed to the metal by the vapor pressure. The expulsion of melt ends with the formation and dispersal of drops with a characteristic size $\sim\sqrt{\chi\tau}$ (see Fig. 1c). Melt is splashed in the direction of the laser pulse. The minimum radiation energy density necessary for splashing of melt by the instability mechanism is ~ 20 J/cm^2.

When the radiation intensity and pulse length vary within the limits indicated above the qualitative picture of the flow of melt is preserved but the quantitative differences (mass of the expelled melt, drop size, characteristic values of the vapor pressure and temperature of the metal) may be fairly large.

3. Under certain conditions the formation of a surface structure on the metal can be initiated by small-scale convection in the layer of melt. When metals are melted by pulsed radiation with $\sqrt{\chi\tau} \ll r_f$ the velocity field has a nonzero vortex component ($\mathrm{curl}\,v \neq 0$), even though the melt moves under the effect of evaporative pressure forces normal to the surface [8]. This is due to the time variation of the thickness of the melt over the focal spot and the low viscosity of the sublayer $\sim\sqrt{\nu\tau}$, which in metals is substantially smaller than the size of the thermal skin-layer ($\sim\sqrt{\chi\tau}$). Small-scale convection is induced in the layer of melt by the evaporative-pressure forces if the characteristic scale of pressure modulation (Λ) does not exceed [8]

$$\Lambda \sim \left(\frac{\sigma}{\rho\sqrt{\chi}}\right)^{1/2} \tau^{3/4}, \tag{6}$$

where σ is the surface tension. Using Eq. (6), we can easily establish that the evaporative-pressure forces will have a decisive effect on the mixing of the melt under irradiation with short laser pulses, no longer than 10 μsec.

The induction of convection by the development of small-scale surface structures was studied in a formulation on the whole coinciding with that used in the analysis of splashing of melt. The main difference was that the boundary conditions were prescribed at the lower limit of the computational region. Besides the condition of a constant temperature, used in Section 2, which is valid at a rather large distance ($\sim 3\sqrt{\chi\tau}$) from the surface of the metal, we considered the condition that there is no thermal flux through the lower boundary, which holds when a metal film is deposited on a thermally insulated substrate. The length of the laser pulses and the radiation intensity were chosen so that the radiation energy density was less than ~ 20 J/cm^2, which corresponds to the condition of splashing of melt.

Figure 3 shows the graphs of the time dependence of various quantities characterizing the formation of a surface relief on an iron film of thickness ~ 2 μm, deposited on a heat-resistant substrate, under radiation of intensity 10^8 W/cm^2. Figure 4 shows the velocity field at two times: in the stage of vortex nucleation in a partially molten film and developed vortex flow. We see from Figs. 3 and 4 that convective processes develop after the laser pulse, which is Gaussian in this case. The evolution of the surface relief is due in this stage to the development of capillary waves with characteristic frequency $\omega \simeq 2 \cdot 10^6$ sec^{-1}, whose value is in good agreement with the value of ω calculated from the familiar dispersion relation for capillary waves

$$\omega = \frac{2\pi}{\lambda}\left(\frac{2\pi\sigma}{\lambda\rho}\right)^{1/2}$$

for perturbations with $\lambda = \Lambda_1$. The characteristic value of the rotational velocity is 0.5 m/sec.

Vortex structures are not observed in thicker metal samples and films deposited on a thermally insulating substrate since the lifetime of the melt is of the same order as the length of the laser pulse.

It is interesting to note that resonance gratings whose amplitudes satisfy the condition for the suppression of specular reflection can be formed during the inertial growth of light-induced surface structures, which is observed after a laser pulse. Figure 4a shows the time dependences of the amplitudes of the Fourier components of a relief with periods Λ_1, Λ_2, and Λ_3 and a uniform component of the absorptivity of the surface under the effect of a Gaussian radiation pulse. In a time ~0.6 μsec the amplitude of the induced resonance grating is maintained at a level 0.1 μm, ensuring a substantial increase in the absorptivity of the surface (~ 20%). In some versions of the calculations the absorptivity of the surface increased to ~60%, which is several times the absorption coefficient of iron with a flat surface.

4. The numerical calculations here on the whole confirm the hypotheses in [3, 4] that splashing of melt and initiation of convection are possible as a result of the development of a surface structure on the melt [8]. The results are in qualitative agreement with the experimental data of other workers [4, 9]. We should note the agreement between the results of our study and the data of Konov et al. [9], who studied the direction of melt splashing as function of the angle of incidence of the laser beam. The results of the numerical calculations are in agreement with the experiment [4], which studied the size distribution of drops in a melt splash caused by single laser pulses. A more detailed quantitative comparison with experiment requires analysis of the effect of a rather large number of parameters, which characterize the space—time and polarization structure of the laser radiation as well as the state of the surface of the material being worked. A quantitative comparison with the experimental data is difficult to make at present because all the necessary information is not available.

NOTATION

Here V is the melt velocity; p is the vapor pressure, ρ is the melt density; t is the time; Λ is the period of the surface structure; τ is the laser pulse length; τ_m is the melt lifetime; χ is the thermal diffusivity; r_0 is the melt drop size; r_f is the focal spot size; λ is the radiation wavelength; h is the grating depth; ε is the dielectric constant of the material; θ is the angle of incidence of the laser beam; ν is the melt viscosity; and A is the uniform component of the absorptivity of the material.

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