Model of deformation of a liquid drop of zirconium dioxide after its collision with a steel porous surface

V V Bublik\textsuperscript{1,2} and A N Cherepanov\textsuperscript{1}

\textsuperscript{1} Khristianovich Institute of Theoretical and Applied Mechanics of the Siberian Branch of the Russian Academy of Sciences, 630090, Novosibirsk, Russia
\textsuperscript{2} Novosibirsk State University, 630090, Novosibirsk, Russia
E-mail: bublik@itam.nsc.ru

Abstract. Based on the integral laws of conservation of mass and energy, a mathematical numerical-analytical model of the deformation of a continuous liquid-metal drop after its collision with a flat porous surface is constructed. The model takes into account the capillary and adhesive properties of the melt, the processes of cooling a liquid drop until it solidifies. Numerical calculations are performed for the model case of collision of a continuous liquid drop of zirconia with a porous steel substrate.

1. Introduction

Investigation of the processes of droplet-substrate collision is given great attention in connection with the tasks of applying protective powder coatings to parts and mechanisms, thermal barrier coatings on turbine blades and aircraft engines, applying solders to microchips, etc. [1–12]. In this case, continuous smooth surfaces are mainly considered. One of the main problems with this is the one of the strength of the coating adhesion to the substrate. In this paper, we study the problem of the interaction of a liquid metal droplet with a porous substrate, which, in our opinion, is of interest from the perspective of increasing the strength of adhesion to the substrate, as well as for issues of dynamic impregnation of working surfaces with various materials resistant to corrosion, chemical and other aggressive influences.

The proposed model is a further development of the models of impact of a solid and hollow drop with a solid substrate [13–15]. In particular, in [14] a mathematical numerical-analytical model of the deformation of a continuous liquid-metal drop after its collision with a flat porous surface in the isothermal case is constructed. The model takes into account the capillary and adhesive properties of the melt. In this paper, this model is generalized to the nonisothermal case.

2. Brief description of the model

Let us describe briefly the model from [14]. The initial diameter of the droplet is $H_0$, the collision velocity of the droplet with the substrate is $v_0$. The initial kinetic and potential energies of the drop are equal

$$W_0 = \frac{\pi \rho H_0^3 v_0^2}{12}, \quad \Pi_0 = \sigma_1 H_0^2.$$
Here, $\sigma_{12}$ is the surface tension at the liquid—gas interface, and $\rho$ is the density of the liquid.

After the collision, we divide the entire volume of the drop into four subregions (see figure 1): $\Omega_g$ is a ball segment formed by rotation around the $z$ axis of curved triangle $hM_1H$; $\Omega_d$ is a disk formed by rotation of rectangle $0hM_1R_c$ around the $z$ axis; $\Omega_T$ is a toroidal region formed by rotation of semicircle $R_cM_1M_2R_c$ around the $z$ axis; $\Omega_s$ is the region of liquid in porous substrate.

The porosity of the substrate will be modeled in the form of vertical capillary tubes. Let $z_s \leq 0$ be the coordinate $z$ of the maximum penetration of the melt deep into the porous substrate (we believe that the maximum penetration depth is achieved on the axis of symmetry of the drop-substrate system). The rate of fluid filtration into the porous substrate is determined from the Darcy equation:

$$\dot{z}_s = \frac{m_s r_p^2 \rho \dot{H}^2}{16 \chi \mu z_s},$$

(1)

where $\chi$ is the tortuosity parameter of the channel, $r_p$ is the effective radius of the capillary, $m_s$ is the porosity of the substrate, $\mu$ is the dynamic coefficient of viscosity of the liquid. We assume that at each moment of time the fluid filtration rate is the same in the entire region $\Omega_s$. From the condition of constant volume of incompressible fluid, we obtain the relation connecting the value of $R_c$ with other parameters of the drop

$$3(H + h)R_c^2 - 6m_s \int_0^t \dot{z}_s R_c^2 d\tau + \frac{3}{2} \pi h^2 R_c + (H - h)^3 + h^3 - H^3 = 0.$$

In each of the subregions $\Omega_g$, $\Omega_d$, and $\Omega_T$, we define our approximation of the velocity field satisfying the continuity condition:

$$u_g = 0, \quad v_g = \dot{H}, \quad u_d = (m_s \dot{z}_s - \dot{H}) \frac{r}{2h}, \quad v_d = (\dot{H} - m_s \dot{z}_p) \frac{z}{h} + m_s \dot{z}_s,$$

$$u_T = (m_s \dot{z}_s - \dot{H}) \frac{R_c^2}{2hr}, \quad v_T = 0.$$

The kinetic energy of a moving fluid will be determined by formula

$$W = \iiint_{\Omega} \frac{u^2 + v^2}{2} - \frac{\rho}{2} d\Omega = \pi \rho \int_{\Omega} (u^2 + v^2) r dr dz.$$
Here, $\Omega$ is the rotation figure formed by rotation around the $z$ axis of the plane region $\Omega_1$. A detailed conclusion and the final form of the formulas for kinetic energies in each of the subregions can be found in [14], and is not given here.

Potential energy of the drop-substrate system is

$$\Pi_\sigma = \sigma_{12}(S_g + S_T + m_s S_d) + (\sigma_{13} - \sigma_{23})((1 - m_s)S_d + S_s),$$

where $\sigma_{13}$ and $\sigma_{23}$ are the surface tension at the liquid—substrate and substrate—gas boundaries, respectively, $S_g = \pi (R_c^2 + (H - h)^2)$ is area of the outer surface of the spherical segment, $S_T = 2\pi h(2h + \pi R_c)$ is area of the lateral surface of the toroidal part, $S_d = \pi R_c^2$ is area of the contact spot excluding porosity, $m_s S_d$ is surface area of the liquid—gas inside the pores (for simplicity we assume that the surface of the liquid in the pores is strictly horizontal), $(1 - m_s)S_s$ is the area of the contact spot taking into account the substrate porosity, $S_s = 2(\pi H_0^3/6 - V_g - V_d - V_T)/r_p$ is the surface area of the liquid—substrate within the pores. The values $\sigma_{12}$, $\sigma_{13}$, and $\sigma_{23}$ are related by formula $(\sigma_{13} - \sigma_{23})/\sigma_{12} = -\cos \theta$, where $\theta$ is the contact angle of wettability.

The work of the adhesion forces when the droplet spreads over the substrate is determined by expression

$$Q = (1 - m_s)\pi R_c^2 \sigma_{12}(1 + \cos \theta).$$

In the disk-shaped region $\Omega_d$, the force of viscous friction acts, therefore, we take into account the work of this force

$$A_\mu = 2\pi \int_0^h dz \int_0^{R_c} F_\mu r dr = \frac{\pi \mu m_s \dot{z}_s - \dot{H} R_c^3}{3h}.$$

Here, $\mu$ is the dynamic coefficient of viscosity of the liquid.

The condition for energy conservation of the drop—substrate system is

$$W_g + W_d + W_T + W_p + \Pi_\sigma + Q + A_\mu = W_0 + \Pi_0. \quad (2)$$

Suppose that the parameters $H$ and $h$ are related by

$$h = H \left(1 - \frac{H}{H_0}\right)^n,$$

where $n$ is the constant chosen to ensure the best agreement with the experiment.

Functions $H(t)$ and $z_s(t)$ are determined from a system of ordinary differential equations (1), (2). As initial conditions, we take

$$H(0) = H_0, \quad z_s(0) = 0. \quad (3)$$

The direct solution of the obtained Cauchy problem causes some difficulties. This is due to the fact that the system of equations is non-linear with respect to the highest derivatives. In previously developed models (with an impenetrable substrate), the highest derivative entered the equation quadratically, which made it easy to isolate the desired branch of the solution from the analysis of the physical model. In the case of a porous substrate, after eliminating $\dot{z}_s$ from equation (2) using (1) we obtain an equation that is a fourth-degree polynomial with respect to $\dot{H}$. In the general case, the roots of the fourth degree polynomial cannot be expressed in an analytical form, therefore, one must either investigate all possible solutions of the Cauchy problem (theoretically, the number of such solutions can reach four), or look for ways to unambiguously single out the highest derivative.
In this paper, we propose instead of the equation on $\dot{H}$ to take its differential consequence

$$A\ddot{H} + B = 0,$$

(4)

where $A = A(\dot{H}, H, z_0)$, $B = B(\dot{H}, H, z_0)$ are known functions that are not given here because of their excessive bulkyness. As the missing Cauchy condition, we take the condition for the drop velocity of the droplet and the velocity of the droplet tip at the moment of collision:

$$\dot{H}(0) = v_0.$$

(5)

Thus, to describe the motion of a droplet after collision with a porous substrate, it is necessary to solve the system of equations (1), (4) with Cauchy data (3), (5).

3. Temperature change simulation

We supplement the droplet spreading model with a description of the process of changing the temperature of a liquid droplet until solidification (we do not affect the solidification process itself). We introduce the effective thermophysical parameters of the region of the substrate impregnated with liquid metal:

$$\lambda_f = \lambda_l m_s + \lambda_s (1 - m_s), \quad c_{Vf} = c_{Vl} m_s + c_{Vs} (1 - m_s),$$

where $\lambda_l$ and $c_{Vl}$ are the thermal conductivity and bulk thermal conductivity of the liquid metal; $\lambda_s$, $c_{Vs}$ are thermal conductivity and bulk thermal conductivity of the substrate material. The drop is cooled due to the radiative heat transfer of its free surface with the surrounding medium with temperature $T_a$ and heat transfer to the substrate with initial temperature $T_{s0}$. In view of the small volume of the droplet, we consider the solidification process volumetric. Then, the heat balance equation in the volume of the drop above the substrate will have the form

$$M(t)c_{Vl}\frac{dT_1}{dt} = -\lambda_f(q - F_1(t)\alpha_r(T_1 - T_a)),
$$

where $M(t)$ is the mass of the melt in the volume of the particle above the substrate; $q = -\lambda_f(\partial T_1/\partial z)$ is substrate heat flux; $T_1$ is liquid metal temperature; $F_1(t) = \pi R_c(t)$ is contact spot area; $F_1(t)$ is free surface of a liquid particle; $\alpha_r = \varepsilon\sigma_0(T_1 + T_a)/(T_1^2 + T_a^2)$ is radiative heat transfer coefficient; $\sigma_0$ is Stefan—Boltzmann constant; $\varepsilon$ is emissivity.

The heat transfer equation in the region of the substrate impregnated with the melt is

$$\rho_f c_{Vf} \left( \frac{\partial T_2}{\partial t} + \dot{z}(t) \frac{\partial T_2}{\partial z} \right) = \lambda_f \left( \frac{\partial^2 T_2}{\partial r^2} + \frac{1}{r} \frac{\partial T_2}{\partial r} + \frac{\partial^2 T_2}{\partial z^2} \right),$$

where $T_2 = T_1 m_s + T_s (1 - m_s)$ is the mass average temperature of the substrate with the melt, $T_s$ is substrate temperature, $\rho_f = \rho_l m_s + \rho_s (1 - m_s)$ is effective density of the substrate with liquid metal.

This equation is solved under boundary conditions

$$T_1 |_{z=0} = T_2 |_{z=0}, \quad -\lambda_f \frac{\partial T_2}{\partial n} \bigg|_{\Gamma} = \frac{\lambda_s}{\phi(t, r)} (T_2 - T_{s0}),$$

where $\phi(t, r)$ is the depth of liquid penetration into the substrate, $\Gamma$ is impregnation boundary. To eliminate the singularity in the denominator of the boundary conditions, we assume that $\phi(t, r) \geq r_p$, that is, we assume that at all points of the contact spot, the liquid penetrates deep into the substrate at least by a thickness of $r_p$. 


Table 1. The dependence of the geometric dimensions of the splat on the temperature of the substrate

| $T_{s0}$, K | $t$, $\mu$s | $-z_s$, $\mu$m | $R_c$, $\mu$m | $H$, $\mu$m |
|------------|-------------|----------------|--------------|-------------|
| —          | 1.9         | 1.5            | —            | —           |
| 1370       | 1.1         | 1.37           | 47           | 19          |
| 970        | 0.95        | 1.29           | 43           | 24          |
| 570        | 0.84        | 1.22           | 41           | 28          |

4. Results of a numerical experiment

We carry out numerical calculations for the model case of collision of a continuous liquid drop of a melt of zirconium dioxide with a porous substrate. The initial diameter of the droplet is 60 $\mu$m, the speed of collision of the droplet with the substrate is 50 m/s, the capillary radius is 0.5 $\mu$m, the porosity of the substrate is 0.15, the tortuosity parameter of channel 1, the metal density is 5600 kg/m$^3$, the surface tension at the interface of liquid and gas is 0.43 N/m, dynamic coefficient of viscosity of the fluid is 0.021 N·s/m$^2$.

The time dependences of the geometrical sizes of the droplet and the region of penetration of the liquid into the substrate are obtained. Calculations show that, without taking into account solidification of the melt, the maximum radius of the contact spot can reach 550 $\mu$m in about 50–100 $\mu$s after the collision. In this case, the maximum penetration depth of the melt into the substrate of 1.5 $\mu$m is reached after about 1.9 $\mu$s. After this, only the drop spreads over the surface.

Different versions of the initial temperatures of the droplet and substrate were investigated. In the calculation, the substrate temperature was taken to be 570 K, 970 K, and 1370 K, and the droplet temperature at the moment of collision was 3300 K. The following thermophysical properties of the zirconium dioxide melt were also used: $\lambda$=3.35 W/(m·K), $T_m$=2960 K, $c$=710 J/(kg·K).

The dependence of the geometric dimensions of the splat on the initial temperature of the substrate is presented in table 1. It turned out that the crystallization temperature of the droplet in all these cases is reached before the maximum penetration of the liquid deep into the substrate. In this case, similar calculations for colliding a nickel drop with a porous steel substrate show that the crystallization of the drop begins only after the drop has completely spread.

5. Conclusion

A numerical-analytical model of the interaction of a metal drop with a porous substrate is constructed. It has been shown that for refractory materials (for example, ZrO$_2$), a higher substrate heating is required to obtain a greater penetration depth.

The proposed solution can be useful for assessing the parameters of the splat when forming powder coatings with dynamic impregnation of porous surfaces in order to harden them and obtain composite layers with improved properties.

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References
[1] Saburov V P, Eremin E N, Cherepanov A N and Minnekhanov G N 2002 Modification of Steels and Alloys with Dispersed Inoculators (Omsk: OmSTU Publ.) (in Russian)
[2] Moskvichev V V, Krushenko G G, Burov A E, Uskov I V and Fedorova E N 2013 Nanopowder Technology in Mechanical Engineering (Krasnoyarsk: Siberian Federal University Publ.) (in Russian)
[3] Orishich A M, Cherepanov A N, Shapeev V P and Pugacheva N B 2014 Nanomodification of Welded Joints in Laser Welding of Metals and Alloys (Novosibirsk: Sib. Branch RAS Publ) (in Russian)
[4] Popov V N and Cherepanov A N 2017 Thermophys. Aeromech. 24 779–86
[5] Cherepanov A N, Mali V I, Malitutina Iu N, Orishich A M, Malikov A G and Drozdov V O 2017 Int. J. Adv. Manufact. Technol. 90 3037–43
[6] Bozhanova N M, Panov I T, Manolov V K, Cherepanov A N and Lazarova R L 2018 Thermophys. Aeromech. 25 759–64
[7] Drozdov V O, Cherepanov A N, Chesnokov A E and Smirnov A V 2018 AIP Conf. Proceed. 2053 030010
[8] Cherepanov A, Cherepanova V, Manolov V and Yovkov L 2018 J. Phys.: Conf. Series 1105 012050
[9] Shapovalov V 1994 MRS Bulletin 19 24–8
[10] Yanagino H, Tsumura T, Nakajima H, Hyun S-K and Nakata K 2006 Mater. Transact. 47 2254–8
[11] Nakajima H 2007 Progr. Mater. Sci. 52 1091–173
[12] Cherepanov A N, Solonenko O P and Publik V V 2009 Thermophys. Aeromech. 15 631–41
[13] Cherepanov A N and Publik V V 2012 Fizicheskaya Mezomekhanika 15 (6) 67–71 (in Russian)
[14] Bublik V V and Cherepanov A N 2018 AIP Conf. Proceed. 2053 040010