Mathematical simulation of particle impact on a fixed surface in the formation of powder coatings

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Abstract. The article deals with the process of elastic and plastic-elastic deformation of the particles during forming of the coating layer. Mathematical model of the process of impacting of powder particle on the fixed surface has been developed. Influence of material properties, kinetic and thermal parameters of deposition on the particle deformation has also been considered.

1. Introduction

Properties of plasma coatings directly depend on their structure. Features of arrangement and structure of plasma coatings, in their turn, depend on material dispersion, heating, acceleration of powder material by the plasma jet, processes of elastic and plastic-elastic deformation of the particles on the basis and development of heterogeneous topochemical interaction of the specific surfaces [1-17].

Mathematical simulation of the processes, heating and acceleration of powder material by the plasma jet are widely represented in [18-19]. In this paper, the research results of the processes of elastic and plastic-elastic deformation of particles during the forming of the coating layer have been presented.

Heated particles of deposited material impact the substrate surface with the speed \( v_0 \), they are deformed and fixed on the surface, and then they are cooled. It is deduced from experiments and confirmed theoretically [3-4] that deformation and cooling of the particle up to the substrate temperature under practically common powder consumption happens individually before approaching the following deposited particles.

To understand the possibilities of the plasma gas-thermal method in providing operating abilities of coatings, it is important to answer the following questions. What is nature, and what factors provide the strength of fixing of particles on the substrate? What factors determine the geometrical shape of the cluster after its fixing on the substrate? What are the possibilities of the process providing the strength of particle fixing on already formed clusters of the structure? What is the influence of residual stresses and deformations on the heterogeneous strength of the coating that is being formed, etc.?

It should be stressed that in spite of numerous research in the sphere of plasma deposition, obtained results are characterized by the research carried out according to the scheme ‘deposition mode – coating property.’ To formulate the problem of forming the coating consisting of clusters of a specific
size, it is necessary to concretize ranges of process parameters, experimental factors used, and to
evaluate the opportunity of realization of some physical processes.

2. Formulation of physical and mathematical model of the process of impacting of powder
particle on a fixed surface

It is assumed that before impacting the surface initial state of the particle is featured by a typical
geometric size $D_0 = 5\ldots100 \ \mu m$, speed $v_0 = 30\ldots100 \ m/s$ and heating temperature $T_{op} = (0,7\ldots1,2) \ T_{melt}$,
where $T_{melt}$ is the melting temperature of particle material. Besides, because of the considered
features of acceleration and heating of particles in a plasma jet such parameters as $v_0$ and $T_{op}$, the
particles at the plasma jet periphery can take values substantially less than for the particles at the jet
axis. It means that it is always necessary to analyze the influence of the dissipation of initial
parameters on the output parameters of the process. Physico-chemical parameters of the particle
depending on the specific material are given for calculating.

Let us consider the schemes of alteration of particle shape on impacting (Figure 1). This scheme of
alteration of particle shape on the surface can be realized practically; stages of such evolution were
fixed by ultrahigh-speed photography [5], and particle parameters after deformation were altered for
various combinations of particle materials and substrates, and various values of $v_0$ and $D_0$.

![Figure 1](image)

*Figure 1. Scheme of alteration of particle shape on the surface hit: a) the stage of impulsive pressure;
b) deformation under forward pressure; c) the final shape of solidified particles.*

It has been ascertained that degree of deformation $k_d$ of initial spherical particles with diameter $D_0$
for about 40 combinations of various materials is altered within [5]:

$$ k_d = \frac{h_k}{D_0} = (0.1\ldots0.05) , $$

(1)

where $h_k$ is the height of the solidified disk (Figure 1).

Consequently, in spite of practically realized a variety of shapes of solidified particles
(undeformed, fragmented into fine fractions, etc.) the structural order of clusters has been shown on
various material combinations.

For quantitative assessment of the structural order, we introduce coefficient of structural order $k$
determined by the relation:

$$ k = \frac{D_k}{h_k} > 1 , $$

(2)

where $D_k$ – diameter of the generated cylindrical disk on the surface (Figure 1). Knowing volume
conservation of the material on spreading, we get that coefficient of structural order (2) with the
deformation degree of the particle (1) is the following:
and for (1) deformation degrees it is altered within $k = (26...74)$, that is, the higher the value $k$ the higher the coefficient of structural order is.

In the cited above paper, it has been experimentally proved that setting (chemical interaction) takes place, not over the whole surface contact area of the cylindrical disk, but over some area of a circle with diameter $D_s$ in the disk center (Figure 1). The ratio of this diameter $D_s$ to the diameter of formed particle $D_k$ for various material combinations is within the range $D_s/D_k = (0.4...0.9)$. However, it is clear that strength of welding of the particle on the substrate is determined by the area, so it is necessary to use as a physical parameter, that determines possible bonding strength, the relation of the mentioned areas, making sense of the relative coefficient of the surface of chemical interaction:

$$k_s = \frac{D_s^2}{D_k^2} = (0.1...0.85)$$

Let us evaluate preliminarily some parameters of the process based on the fact that further calculations will be checked up, and according to the verification principle considered mathematical models will be assumed or checked.

Let us evaluate magnitude of heating due to the conversion of a part of its kinetic energy into heat. Taking into account that heat $Q$ received by the particle is to meet the requirement $Q < (mv_o^2/2)$, where $m$ is a particle mass; $Q = m \cdot c \cdot \Delta T$ where $c$ is its heat capacity, it will have the following relation for temperature rise:

$$\Delta T < \frac{v_o^2}{2c}$$

Relation (5) for $v_0 \leq 250$ m/s and $c = 10^3$ J/kg K gives $\Delta T < 31$ K. The obtained value is not able to change substantially temperature of the particle $T_{02} \approx T_{melt}$, but it can play the role in more sensitive processes connected with the crystallization of multi-component melt of particle material.

Let us evaluate minimum particle rates $v_0$, at which it is possible to reach watched deformation degrees (1). Besides, it is supposed that all kinetic energy is spent on the increase of its surface when transforming a ball into a flat disk:

$$\frac{2m v_o^2}{\alpha} > (S_e - S_o) \alpha,$$

where $S_e$ and $S_o$ are surface areas of the disk and the ball respectively; $\alpha$ is the specific surface energy (surface tension) of the particle material. Transforming this relation, we get:

$$v_o > \left[ k^2 + \frac{6k^2 \rho - 3}{\rho D_o} \right]^{1/2}$$

where $\rho$ is the density of particle material.

Taking into account that for nickel melt $\alpha = 1.62$ N/m and $\rho = 8.9 \cdot 10^3$ kg/m$^3$, the deformation degree, for example, $k_d = 0.07$ is possible at rates $v_0 > 12$ m/s, and $v_0 > 43$ m/s for the particles with $D_o = 60 \mu m$ and $D_o = 5 \mu m$ respectively. These rate values are easily realized on plasma deposition, but it is seen from the calculation that in the case of particle deposition with a wide range of $D_o$ or in case of impact the particles from the peripheral part of the plasma jet on the surface, undeformed particles can be watched in the coating.

The formation of chemical bonds between the deposited particle and the substrate is to meet welding processes in the solid phase or soldering and to involve the following stages: the formation of a physical contact of the particle with the substrate, plastic deformation of the particle, cooling the system of particle-substrate, crystallization of the particle, rise of residual stressed-deformed state in the system, development of volumetric interaction.

However, in contrast to welding, deposition processes are characterized by a very short timing cycle. This results in some principal differences. To characterize these differences, it is necessary to estimate the duration of the processes mentioned above.
To estimate what state – melted or solid – deformation of an initially melted particle is taking place, we evaluate its crystallization time \( t_{cr} \) based on the relation:

\[
t_{cr} = \frac{h^2}{a_1 (2 \beta)}
\]

where \( h \) is the thickness of the cluster melt, \( \beta \) is the root of the characteristic equation, \( a_1 \) is the thermal conductivity coefficient of particle material.

Taking into account that \( \beta \approx (0.4…0.8) \) in a wide range of materials and temperatures \( h \approx 0.1 \ D_0 \), \( a_1 = 1.7 \times 10^{-5} \text{ m}^2/\text{s} \) and \( a_1 = 6.5 \times 10^{-7} \text{ m}^2/\text{s} \) for nickel and zirconium dioxide, we get for the particles with the diameter \( D_0 = 40 \ \mu\text{m} \) crystallization time for nickel \( t_{cr} = 6.5 \times 10^{-7} \text{ s} \) and for zirconium dioxide \( t_{cr} = 1.7 \times 10^{-5} \text{ s} \).

The cooling time of these particles from the melting temperature to the substrate temperature \([3]\) is \( t_{cool} \approx t_{cr} \).

The impact of a particle on the substrate is connected with excitation of a shock wave in the particle material and plastic deformation (spreading) of the particle under the action of its kinetic energy. Let us estimate the actions of these factors. The shock wave spreads in the particle material at the speed of sound that is \( v_s = 3 \times 10^3 \text{ m/s} \) for the melted particle. So, the action time of impact pressure is calculated as:

\[
t_s \leq \frac{D_0}{v_s} \approx 10^{-4}
\]

Consequently, the process of shock wave spreading lasts for much less time than the time of particle solidification. This process is to be considered as a wave spreading in the particle material and as a substrate in adiabatic conditions.

The role of interaction processes for forming of strong bonding of the particle with the substrate was unreasonably belittled until their crucial role in the activation of contact surface has been ascertained \([5]\). It has been shown that stresses arising in the area of particle impact the substrate surface contribute to the emergence of dislocations on the contact surface and activate the setting due to breakage of saturated bonds of solid body atoms. Actually, because of the emergence of dislocations on the surface, a certain density of active centers is developed on it, and the setting of material happens in these centers. It has been experimentally ascertained that initially existing dislocations on the surface are not setting centers, moreover, they prevent setting. In particular, ascertainment of these facts required a certain correction of view of mechanical treatment applied to activate the surfaces before coating deposition.

The density of the emergence of dislocations on the surface rises with the increase of particle rate (their kinetic energy), but an increase of this rate beyond certain limits results in the dispersion of particles and decreasing of operating abilities of coatings.

Dispersion of melted particle impacting solid surface in hydrodynamics is connected with buckling of spreading front of particle material. It is evaluated by Weber criterion \( We \) (inertia force to capillary force ratio):

\[
We = \frac{\rho v^{1/2} l}{\alpha}
\]

where \( v \) is the material flow rate of the particle; \( l \) is the layer thickness where buckling happens; \( \alpha \) is specific surface energy of the melt (surface tension).

It is seen from (9) that increase \( v \) and \( l \), and decreases \( \alpha \) contribute to the dispersion of the particle. Now there are no clear criteria of this process for melted particles with \( D_0 = 5…100 \ \mu\text{m} \), and estimation of the process is carried out based on experimental facts.

An important experimental fact discovered during the impact process and the following deformation of melted particles is that until the last spreading moment of the particle its upper part does not ‘feel’ deformation of its lower part at the point of contact of its surface with the substrate. The upper part of the spherical particle remains its spherical shape, and each part of this surface goes
on moving at the rate of the particle up to the hit [5]. This fact allows us to evaluate the transformation time of a spherical particle into a flat disk based on the relation:

\[ t_e = \frac{D_0 - h_1}{v_0} = \frac{D_0(1 - k_x)}{v_0} \]

(10)

For example, for the particles with \( D_0 = 40 \, \mu m \), \( v_0 > 60 \, m/s \) obtained value of deformation time \( (t_e < 6 \times 10^{-3} \, s) \) is less, but in some cases it can be close to the crystallization time of the particle, that is melted particles are deformed in liquid state and then crystallized. Consequently, for the melted particles, processes of deformation and structural order are considered at a constant temperature, and crystallization is considered as a movement of the crystallization front in the cylindrical disk. If the particle in the initial state is not melted, the possibility of independent consideration of deformation dynamics and temperature equalization is determined by Pecklet number \( Pe \) that is the temperature equalization time in the system \( t_e = D_0^3/a \) to the deformation time ratio:

\[ t_e = \frac{D_0}{v_0}, \quad Pe = \frac{D_0 v_0}{a} \]

(11)

where \( a \) is thermal diffusivity of the particle.

For the typical values of the process \( D_0 \approx 50 \, \mu m \), \( v_0 > 40 \, m/s \); \( a \approx 10^6 \, m^2/s \) Pecklet number \( Pe \gg 1 \), this gives an opportunity of independent consideration of the impact and deformation processes at some value of constant temperature and processes of the following heat-transfer in already deformed particle.

Thus, conducted analysis and estimations of the process allow us to conclude that it is possible to consider unrelated tasks of wave propagation, deformation, spreading, heat-transfer, chemical bonding principally and greatly decreases labor intensiveness of mathematical simulation. It also allows obtaining rather precise estimates of the process analytically.

3. Mathematical simulation of the process of impacting of powder particle on the fixed surface

The impact of the particle on the substrate surface corresponds the sudden force applied to the contact point. The action of these suddenly applied loads spreads into the material of a solid body not instantly (the static task of mechanics of deformable media), but happens wavily (dynamic tasks of mechanics of deformable media). The essence of this wavy perturbation can be represented in the following way.

Displacement \( U \) points of material under external loads results in deformation \( \varepsilon \) of material and consequently, stress \( \sigma \). Arisen stresses result in displacements of closely located points of material, etc. Transfer of this perturbation in the material is described by the dynamic equation [20]:

\[ \rho \dddot{U}_i = \frac{\partial \sigma_{ij}}{\partial x_j}, \]

(12)

where \( \dddot{U}_i \) means double time differentiation of components of displacement vector \( U_i \), and repetitive index \( \kappa \) in the right part means the summation of this index.

Substitution into (12) instead of the stress tensor of physical medium equations describing the interrelations of stresses with deformations instead of Cauchy relations results in the fact that displacement vector satisfies the wave equation.

For the case when the displacement vector of the isotropic medium is a function of only one of the coordinates, for example, \( x \) (flat wave) these equations for the components of the displacement vector are the following:

\[ \frac{\partial^2 U_i}{\partial x^2} - \frac{1}{c_i^2} \frac{\partial^2 U_i}{\partial t^2} = 0, \quad \frac{\partial^2 U_i}{\partial x^i} - \frac{1}{c_e^2} \frac{\partial^2 U_i}{\partial t^2} = 0, \]

(13)

where \( i = x, z, \ c_i = \sqrt{\frac{E}{(1 - \mu)\rho(1 + \mu)(1 - 2\mu)}}, \ c_e = \sqrt{\frac{E}{\rho(1 + \mu)}} \), \( E \) is Young modulus, \( \mu \) is Poisson ratio.

Consequently, the external effect in an elastic medium is transferred by the spreading of independent waves. In one of the waves, displacement is directed along the spreading of the wave.
itself (longitudinal axis) with rate \( c_l \). In another, the displacements such as \( U_{xy} \) and \( U_z \), are directed in the surface perpendicular to the spreading direction (lateral axis) of the wave with rate \( c_l \).

It is known [20], that volume alteration under deformation is determined by the diagonal term sum of deformation tensor \( \varepsilon_{ii} = \text{div} \vec{U} \), that is why in the lateral wave is \( \text{div} \vec{U} = 0 \), and lateral wave spreading is not connected with volume alteration of solid body areas. In longitudinal waves, the spreading is accompanied by compression and expansion of the material in the body.

In reality, a situation collision of bodies does not happen momentarily, but for a certain period connected with contact area increase (the physical approach of the materials) and growth of particle displacement at the boundary. In this case, starting from the fact that in each time moment of the interaction of bodies, simple wave arises because of momentary displacement (13), and their combined action is determined by superposition of such solutions connected with integration simple waves over the action time of this contact material deformation.

In the cases when the collision of solid bodies results in a transfer from elastic to plastic-elastic region of material deformation as deformation increases, plastic-elastic waves rise at the front of wave displacement. Rate of spreading of plastic-elastic waves at a first approximation is determined by the same relations as in case (13), but instead of Young modulus \( E \), there is \( E_l = d\sigma/d\varepsilon < E \) determined from real deformation dependence of the material.

It follows that the rate of the plastic-elastic wave is less than the rate of elastic wave in the same material. However, it is necessary to keep in mind that deformation dependencies \( \sigma = \sigma(\varepsilon) \) for the cases of static (slow loading) and dynamic loading substantially differ from each other. First, under dynamic loading deformations depend not only on deformation value \( \varepsilon \), but deformation rate \( \dot{\varepsilon} \). Therefore, multiple experimental pieces research have ascertained that the yield strength of some soft metals under dynamic loading can reach values 2-3 times higher than under static loading.

Let us consider the task if impacting and spreading of a drop in stages, and we start with a situation analysis of its elastic deformation. Because of the spreading rate of elastic waves in the ball \( c_s > v_0 \) we neglect its elastic vibration and consider the task of impact in a static problem statement.

It is known [20], that alteration of the potential energy of the ball when approaching a flat perfectly rigid surface by value \( h \) (the difference between \( D_h \) and distance from an upper point of the ball to the surface) under elastic deformation is determined by the equation:

\[
U = h^2 A_u, \tag{14}
\]

where \( A_u = 8E\sqrt{B_0}/15\sqrt{2}(1-\mu^2) \).

During the impact time, the total energy of the ball is a sum of the kinetic energy \( m(h)^2/2 \) and the potential one (14). According to the energy conservation law (region of elastic deformations), we get the equation of ball motion in the form of:

\[
\left( \frac{dh}{dt} \right)^2 + Ah = v_0^2 \tag{15}
\]

\[
A = 32/9\pi\sqrt{2}(1-\mu^2)D_0^{5/12} \rho \tag{16}
\]

Applying the relation to the rate of longitudinal elastic wave (13) represent (16) in the form of:

\[
A = \frac{32}{5\pi}\sqrt{2}(1-\mu^2) \frac{c_l^2}{D_0^{5/12}} = A_u \frac{c_l^2}{D_0^{5/12}} \tag{17}
\]

The maximum approach of the ball with the surface \( h_0 \) happens at the time moment when its rate \( h \) equals zero. That is why from (15) we get:

\[
h_0 = \frac{D_0}{A_u^{1/5}} \left( \frac{v_0}{c_l} \right)^{4/5} \tag{18}
\]

Then the impact time (the period when \( h \) alters from 0 to \( h_0 \) and inversely up to zero) will be:
Calculating the obtained integral we get:

\[
t = 2 \int_0^{h_0} \frac{dh}{\sqrt{h_0^2 - Ah_0^{3/2}}} = 2 \left[ \frac{1}{A^{1/2} v_0} \right]^{1/3} \int_0^{1} \frac{d\xi}{\sqrt{1 - \xi^{2/3}}} \]

From the obtained equation, it is seen that the time of elastic collision slightly depends on the ball rate; it is practically determined by the period of spreading of the elastic wave from the lower to the upper point and back.

To describe the plastic deformation of a particle, and to simplify the calculation, let us assume it as a cylinder rod of initial length \(h_0\) and sectional area \(S_0\). Rod with initial rate \(v_0\) impacts perfectly rigid substrate and it is deformed on it. Let us know the curve of uniaxial compression of the material \(\sigma = \sigma(\varepsilon)\), and the plastic flow of the material starts with some value \(\sigma = \sigma_s\).

If the front of plastic wave deformation spreads from the fixed surface with the rate \(v_p(t)\) and leaves behind stationary material, and above the material moves as a solid body with decreasing rate \(v(t)\).

Because of the incompressibility of the material:

\[
(\varepsilon + v_p)S_0 = v_p(t)S_p(t) \tag{20}
\]

It is seen from this condition that at the front of the plastic wave, the cross-sectional area is to change unevenly from \(S_0\) to \(S_p\)- cross-sectional area of the material behind the wavefront.

Material deformation behind the wavefront is calculated in the following way: some column of undeformed material with length \(v + v_p\) transfers in the column of deformed material with length \(v_p\) in a unit of time. So,

\[
\varepsilon = -\frac{v_p - (v + v_p)}{v + v_p} = \frac{v}{v_p + v} \tag{21}
\]

We designate \(h(t)\) the length of the undeformed part of the sample at the time moment \(t\). Then

\[
-\frac{dh}{dt} = v + v_p \tag{22}
\]

When the wave front passes through the element of the rod \(dx = -dt(\varepsilon + v_p)\) the rate of this element becomes zero. Applying momentum conservation law, we get:

\[
\rho \left(\varepsilon + v_p\right)S_0 dt \cdot v = S_0 \left(\sigma - \sigma_s\right) dt \]

or

\[
\rho \left(\varepsilon + v_p\right) v = \sigma - \sigma_s, \tag{23}
\]

where \(\sigma\) - stresses in the elastic region of the rod.

Let us compose an equation of motion of undeformed rod part taking into account its variable length \(h(t)\), and in front of the material front it transfers into the plastic state, that is, it is pressed by the force \(\sigma_s S_0\). Consequently,

\[
\rho h \frac{dv}{dt} = -\sigma_s \tag{24}
\]

Applying (21) and (22) we get that

\[
dt = -\frac{\varepsilon dh}{v},
\]

Applying (23) and (21) we get:

\[
\rho v^2 = \varepsilon (\sigma - \sigma_s) \tag{26}
\]

Consequently, the relations (26) and (25) allow getting the differential equation with separating variables:
\[ d \left[ e (\sigma - \sigma_s) \right] = 2 \sigma_s v d (\ln h) \]  

The solution of this equation is carried out at initial conditions:

\[ h = h_0, v = v_0, \sigma = \varepsilon_0, \quad t = 0, \]

where \( \varepsilon_0 \) is determined from (26)

\[ \rho v_0^2 = \varepsilon_0 (\sigma_0 - \sigma_s), \quad \sigma_0 = \sigma (\varepsilon_0) \]

Solving (27), we get:

\[ \ln \frac{h}{h_0} = \frac{1}{2 \varepsilon_0} \int \frac{d \left[ \frac{\varepsilon}{\sigma_s} - 1 \right]}{\varepsilon} \]

4. Results and discussion

Thus, using chosen and experimental dependence \( \sigma = \sigma (\varepsilon) \) from (29) we determine \( \varepsilon = \varepsilon (h) \) deformation depending on \( h \). From (26) we find \( v = v (h) \) the rate depending on \( h \), and from (21) – rate \( v_p = v_p (h) \) of the front of the plastic wave as a function \( h \). After that from (22), we define \( h \), as a function of time. The final shape of the deformed particle is found from the condition (24) when the left part of the relationship reaches the value \( \sigma_s \) that meets the stoppage of particle transformation.

5. Conclusions

The mathematical model of the impact and deformation of a particle of deposited material in the cluster of coating structure on the impact on the substrate has been developed. Regularities of such deformation depending on material properties, kinetic and thermal parameters of the deposition process have been revealed. It has also been ascertained that the time of elastic collision slightly depends on the particle rate, and it is practically determined by the time of spreading of the elastic wave from upper to lower point and back.

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