PROCEEDINGS OF THE INTERNATIONAL CONFERENCE
NANOMATERIALS: APPLICATIONS AND PROPERTIES
Vol. 2 No 3, 03PISERE03 (4pp) (2013)

Computer Simulation of Temperature Profiles for DC Pulse Plasma Jet Modification of Co-based Plasma Detonation Coatings

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(Received 19 May 2013; revised manuscript received 17 July 2013; published online 30 August 2013)

This paper deals with locating the temperature field in a coated plate heated by a moving heat source. The relevance of this problem lies in the challenge of selecting the optimum exposure modes for modifying irradiation of protective powder coatings deposited by a high-speed plasma jet. Based on a number of experimental studies of the structure and properties of these coatings before and after additional plasma jet irradiation, we concluded that it is necessary to model the distribution of temperature during irradiation in order to justify the choice of irradiation parameters such as the source power density and speed. The values and the distribution of temperature in depth from the surface heated by the source play a crucial role in reducing the particles of strengthening phases from the solid solution and accelerating diffusion processes between the coating and the substrate. Comparing the experimental data with the calculations of the temperature profile, we can offer the best exposure modes, which do not lead to excessive heating of the coating, but result in changes in the phase composition and the improvement of adhesion of the coating with the substrate by accelerating the diffusion processes between the coating and the substrate.

Keywords: Temperature Profile, Mathematical Modeling, High-Speed Plasma Jet, Protective Powder Coatings.

PACS numbers: 07.05 – t., 81.05.Bx

1. INTRODUCTION

The efficiency of advanced technology of getting protective coating by means of pulsing plasma jet deposition of Co-based powders onto steel items often falls due to the porosity of the received coatings and their poor adhesion to the substrate [1, 2]. To eliminate these disadvantages the coatings are modified by the plasma jet or electron beam [1]. The processes of diffusion and formation of new phases in materials under the influence of electron irradiation happen very quickly, the temperature being one of the main factors influencing these processes. However the temperature measurement under irradiation conditions is difficult and unreliable. Development of a mathematical model of temperature distribution in a material depending on irradiation parameters makes it possible to assume the kind of structures and phases that form in the material during irradiation (on the basis of the received values of temperature and the known phase diagrams).

We need to provide the choice of duplex treatment modes according to the energy of plasma jet, time of action on surface, etc. Therefore we need a correct model of a structure-phase composition of a coating before additional treatment. On the basis of this model we may recommend additional irradiation modes.

This paper deals with locating the temperature field in a coated plate heated by a moving flat axisymmetric heat source. Based on a number of experimental studies of the structure and properties of these coatings before and after additional electron beam or plasma jet irradiation [3], we concluded that it is necessary to model the distribution of temperature during irradiation in order to justify the choice of irradiation parameters such as the source power density and speed. The values and the distribution of temperature in depth from the surface heated by the source play a crucial role in reducing the particles of strengthening phases from the solid solution and accelerating diffusion processes between the coating and the substrate. Comparing the experimental data with the calculations of the temperature profile, we can offer the best exposure modes, which do not lead to excessive heating of the coating, but result in changes in the phase composition (the formation of strengthening particles) and the improvement of adhesion of the coating with the substrate by accelerating the diffusion processes between the coating and the substrate.

2. EXPERIMENT

2.1 Modeling of Temperature profiles

The problem of modeling temperature profiles in the modification of properties of coatings by irradiation leads to the following problem in the theory of heat conduction: there is a composite solid body consisting of a plate made of a material with known thermophysical properties (substrate) that is in contact with the plate (coating), made of a material also with well-known thermophysical characteristics, different from the analogous characteristics of the substrate. The coating thickness will be denoted by h. The thickness of the substrate will be $H>>h$ (the coating thickness is approximately $h = 2 \times 10^{-4} \div 6\times10^{-4}$m at the thickness of the substrate $h = 1 \times 10^{-2} \div 2 \times 10^{-2}$ m). The coating surface

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is heated by a moving beam of electrons, which is modeled by a flat axisymmetric heat source, whose surface power density at a point located at distance r from the axis of the beam is defined by the function $Q(r)$. Under computation $Q(r)$ was assumed Gaussian $Q(r)=A\times exp(-(\sigma r)^2)$, whose parameters are determined by the power and the effective diameter of the beam. In the systems for irradiation the heating spot makes a zigzag path on the coatings surface which provides even heating of a sample. Although the modeling of the source traveling by a complex trajectory is quite possible, in practice one can greatly simplify the task by considering the mode of thermal saturation that occurs when driving a flat source along a straight line with constant speed. Indeed, in the coordinate system moving together with the source, after some time from the beginning of the action of the source is set the mode at which the temperature of each point of the sample will depend only on the coordinates of this point (but not on the time). With the plates of generous size and relatively low speeds of the beam this mode of heat saturation will operate most of the processing time. In the case when the thermal properties of the coating and the substrate do not depend on the temperature, the task, as will be shown, can be reduced to the following problem of the theory of heat conduction with a stationary source: Let a heat source on the surface of the coated plate turn on at the initial moment of time; its power density is described by the formula (1)

$$N(r,t) = Q(r)\times\eta(t) \qquad (1)$$

Where

$$\eta(t) = \begin{cases} 0, & t<1 \\ 1, & t\ge 0 \end{cases} \qquad (2)$$

We must find the temperature field $T(r,z,t)$ in the cylindrical coordinate system, the axis of which coincides with the axis of the source and is directed inwards the plate. It is shown that having solved this problem, we can find the field of the moving source by computing quadratures. We introduce the Cartesian coordinate system, whose plane xy coincides with the plane of the plate, and whose axis z is directed inwards the plate. It is assumed that the heat source is turned on at the time $t=0$, where at the initial moment the axis of the source passes the point S located on the surface of the plate with the coordinates $S(x_0,00)$ and moves along the axis x at a speed of v. In this case, we can find the temperature T_A at the point $A(x,y,z)$ at the moment t by applying the principle of superimposition. It is easily shown

$$T_A = \int_0^t \left(\frac{\partial T\left(\sqrt{(x_0-u\times\tau)^2+y^2}, z, \tau\right)}{\partial\tau} \right) d\tau \qquad (3)$$

To find the function

$$T_d(r,z,t) = \left(\frac{\partial T(r,z,\tau)}{\partial\tau}\right)_{\tau=t}$$

we have considered the following problem of thermal conductivity: there is a composite solid body which is a semi-infinite cylinder of radius R (area of space defined by the inequalities $r\le R$, $z>h$), filled with a material with the heat transfer coefficient k_2 and the coefficient of thermal conductivity a_2, which contacts with the cylinder of radius R and height h, made of a material with the heat transfer coefficient and the coefficient of thermal conductivity k_1 and a_1 respectively. At the initial moment of time a plane axisymmetric heat source starts acting on the surface of the body; its surface power density is given by the function $N(r,t) = Q(r)\times\eta(t)$; at that, the temperature of the side surface of the composite cylinder is kept at zero. The temperature of the body at the initial moment is zero. Find the temperature field of the upper cylinder given by the function $T_1(r,z,t)$, defined in the field $(0\le r\le R,\ 0\le z\le h)$ and the temperature field in a semi-infinite cylinder – function $T_2(r,z,t)$ defined in the field $(0\le r\le R,\ z<h)$. We are entitled to assume that if the function $Q(r)$ is finite, i.e. there is such r_{max}, that $Q(r)=0$ if $r>r_{max}$, and $r_{max}<<R$, then resolving this problem will be a good approximation to the field $T(r,z,t)$. The above problem is a boundary value problem of determining functions $T_1(r,z,t)$ and $T_2(r,z,t)$, satisfying certain boundary initial conditions and the differential equations of heat conduction. The function $Q(r)$ is approximated by the first N terms of its Fourier-Bessel expansion in Bessel functions $J_0(r)$:

$$Q(r) \approx \sum_{k=0}^{N} a_k J_0(\zeta_k r) \qquad (4)$$

where $\zeta_k = \lambda_k / R$ (λ_k - kth root of the function $J_0(r)$). The solution of the problem will be

$$T_1 = \sum_{k=0}^{N} a_k T_{1k} \qquad (5)$$

$$T_2 = \sum_{k=0}^{N} a_k T_{2k} \qquad (6)$$

where the functions T_{1k} and T_{2k} satisfy the differential equation of heat conduction,

$$\Delta T_{1k} = \frac{1}{a_1}\frac{\partial T_{1k}}{\partial t} \qquad (7)$$

$$\Delta T_{2k} = \frac{1}{a_2}\frac{\partial T_{2k}}{\partial t} \qquad (8)$$

the boundary conditions,

$$k_1\left(\frac{\partial T_{1k}}{\partial z}\right)_{z=0} = -\eta(t)\, J_0(\zeta_k r) \qquad (9)$$

$$k_1\left(\frac{\partial T_{1k}}{\partial z}\right)_{z=h} = k_2\left(\frac{\partial T_{2k}}{\partial z}\right)_{z=h} \qquad (10)$$

$$T_{1k}(r,h,t) = T_{2k}(r,h,t) \qquad (11)$$

as well as the condition $T_{2k}(r,\infty,t)=0$ and initial conditions $T_{1k}(r,z,0)=0$ and $T_{2k}(r,z,0)=0$.

The functions T_{1k} and T_{2k} are found with the help of applying the Laplace transform with respect to the variable t. The authors propose a mixed (numerical and analytical) method for finding the original of the Laplace transform T_{1k} and T_{2k} by their known images $\overline{T}_{1k}$ and $\overline{T}_{2k}$. We implemented a program of calculations. The user interface allows obtaining three-dimensional graphs of the temperature distribution in the depth of two-layer metal absorbers along with the data entry on the parameters of the moving source.

2.2 Experimental Details

150 -300 μm thick protective coatings were deposited on steel substrate with an "Impulse-6" plasma detonation unit. The substrate material was stainless steel 3 (Fe – base, C - 0.25 %, Mn – 0.8 %, Si – 0.37 %, P < 0.045 %). For the coatings we used the AN-35 Co-based powder alloy with additives of Cr (8…32 %); Ni (≤ 3 %), Si (1.7…2.5 %), Fe (≤ 3%); C (1.3…1.7 %) and W (4…5 %). The size of powder fractions varied from 56 to 260 μm. The substrate surface was pre-treated by sandblasting. The size of the steel samples was $20\times30\times10$ mm^3. The powder coatings deposition was carried out in air by the following modes: the distance from the sample to the plasma jet nozzle edge – 60 mm; sample velocity – 360 mm/min; pulse frequency – 4 Hz. The electric current density in a plasma jet can vary from 1 to 7 A/cm^2; the heat transmission rate in the sample varies in the q = (0.1…5) 10^6 W/cm^2 depending on the electric current density; the average temperatures of the plasma flow at the nozzle exit of the installation reach the order of several thousand ˚C; the average diameter of a plasma jet on a sample is 25 mm; pulse duration of the order of 10 μs [1; P.374-379]. For combustion we used propane, oxygen and air, while Mo was selected as a plasma-jet eroding electrode material.

The coating was deposited and the additional treatment was produced at the Sumy Institute for Surface Modification (Sumy, Ukraine). The modes of additional irradiation by DC pulse plasma jet: power density of plasma jet is 1.9×10^9 W/m^2; pulse duration is 3×10^{-6} sec; pulse frequency is 2.5 Hz. Selecting the power density of the plasma jet to cover the additional processing is based on the results of mathematical modeling of the temperature profile in the double-layer absorbers described in Section 2 of this paper.

Experimental methods of analysis: Atomic Force Microscopy (AFM) by JSPM-5200 ("JEOL", Japan) and by NT-206 (Belorussia), Transmission Electron Microscopy (TEM) by JEM-2100 ("JEOL", Japan), Scanning Election Microscopy (SEM) by JSM-6390LV ("JEOL", Japan) with Energy Dispersive Spectrometry (EDS) ("Oxford Instruments", Great Britain), X-ray diffraction (XRD) by X'Pert PRO ("PANalytical", the Netherlands). The foils for TEM were prepared by the Ar ion sputter etching method using the Precision Ion Polishing System –M-691 ("Gatan", USA). For a more detailed analysis of the coating, it was mechanically cut off the surface of the substrate to examine the structure at different depth from the coating surface.

Because the thickness of the coatings is from 150 to 300 microns, we applied different methods to investigate the structure, element composition and mechanical properties of the coatings at different depths. Thus we investigated different coat layers.

Microhardness was measured on the angle laps of coatings using PMT-3 microhardness meter (LOMO, Russia) with an indentation load of 2, 5, and 10 N.

3. RESULTS AND DISCUSSION

The surface of plasma-detonation coatings is highly rough. The average roughness coefficient Ra is 100 nm. Not fully melted powder particles of the coating are visible on the surface.

The phase structure of the coatings differs with the depth (see Table 1). The reduction of γ- phase parameter a with depth was noted in the coatings. In the interface (coating layers that contact the substrate) the Fe–based phase volume concentration rises (taking into consideration that Fe is the basic component of the substrate); and the oxides disappear. TEM proved that the base through-thickness layer of plasma detonation coatings presents a mixture of crystallographically differently oriented nanograins of Co-based solid solution (fcc) with the size of 50 nm and lamellas of intermetallic phases up to 50 nm long and 5 nm in diameter (Fig. 1a). The indexed reflexes of intermetallic phases (Fig. 1b) were tested by the dark field method (see Fig. 1c). Apparently, it is a $Co_{0,8}Cr_{0,2}$ - phase. The data about existence of a phase with a hexagonal lattice in the Co-Cr binary system was first published in data [4], the data about its structure was published in data [5].

The phase composition of a coating after irradiation according to the design conditions changes; the volume fractions of Co-based solid solution and intermetallic phase increase (see Table 1). Mo appears on the surface of a coating after irradiation under the estimated regimes (Table 1).

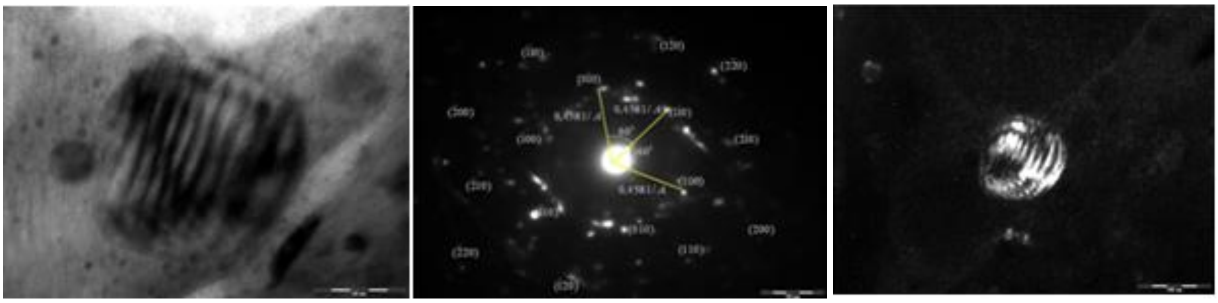
After further treatment by a plasma jet the adhesion of the coating to the substrate significantly increased, thus making it hard to mechanically cut the coating from the substrate, unlike prior to irradiation. A too thick layer of the steel substrate is taken when cut off. Therefore, Table 1 shows the data obtained only in the analysis of the irradiated coating surface. Microhardness of a coating increases; the width of the diffuse zone increases (Fig. 2). The roughness decreases at the expense of melting the coating surface, which corresponds to the specified temperatures at the surface of the coating. The average value of roughness coefficient Ra of a coating after irradiation is 53 nm.

The formed structures are stable at room temperature, no reduction of strength properties is observed. We consider that the nano-sized lamellae of $Co_{0.8}Cr_{0.2}$ intermetallic phases are reinforcing, since the microhardness of plasma-detonation coatings varies with depth and correlates with the volume fraction of the phase irradiated electrode and the increase of the width of the diffuse zone in the coating layer contacting the substrate (Fig. 2 and Table 1). It is evident that molybdenum penetrates the surface from the Mo electrode.

Our results are in good agreement with the data of other authors, who note, firstly, the formation of a polycrystalline matrix of crystallographically disoriented nanograins in films [6] and in protective coatings [7], including plasma-detonation coating [8]; secondly, notice the radiation-enhanced diffusion in materials with an fcc lattice during irradiation, leading to heating up to the temperatures we specified [9].

Table 1 – Phase composition of the Co based coating and substrate

№	Material and the field of analysis	Volume concentration. Chemical formula. Crystal system. Space group. Space group number. Parameters (Å)
1	AN-35 base powder	20 vol.% - Co –based solid solution, hexagonal (hcp); 70 vol.% - Co –based solid solution, cubic (fcc); 10 vol.%- $CoCr_2O_4$, cubic (fcc), Fm-3m (225), a=8.2990
2	coating AN-35 0-50 μm from surface	60 vol. % - Co-based solid solution, cubic (fcc), Fm-3m (225), a =3.55…3.54 ; 15vol. % - $Co_{0.8}Cr_{0.2}$, hexagonal, P63/mmc (194), a =2.52; b = 2.52; c = 4.062; 10 vol. % $FeCr_2O_4$- cubic (fcc), Fm-3m (225), a =8.3780; 15 vol. % CoO- cubic (fcc), Fm-3m (225), a =4.2200
3	coating AN-35 100-150 μm from surface	50 vol. % - Co-based solid solution, cubic (fcc), Fm-3m (225), a =3.52-3.53; 15 vol. % - $Co_{0.8}Cr_{0.2}$, hexagonal, P63/mmc,194, a =2.52; b = 2.52 ; c = 4.062; 35 vol. % CoFe– cubic, Pm-3m, 221, a =2,8570
4	coating AN-35 after added irradiation by direct current pulse plasma jet 0-50 μm from surface	70 vol. % - Co-based solid solution ,Cubic (fcc), Fm-3m, a =3.5(4); 20 vol. % - $Co_{0.8}Cr_{0.2}$, hexagonal, P63/mmc, a =2.52; b = 2,52: c = 4.062; 3 vol. % - $FeCr_2O_4$- Cubic (fcc), Fm-3m (225), a =8.3780; 7 vol. % - Mo, Cubic, Pm-3m a=3.130 and MoO2 and MoO_3



a b c

Fig. 1 – TEM - images of AN-35 coating: the $Co_{0.8}Cr_{0.2}$ particle, bright field (a); an electron diffraction pattern of a $Co_{0.8}Cr_{0.2}$ particle, the zone axis is [001](b); the Co $_{0.8}$Cr $_{0.2}$ particle (dark field) shot in point reflex (010) (c)

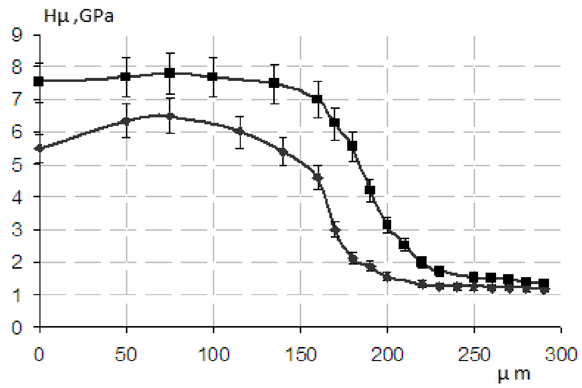


Fig. 2 – The curves of distribution of microhardness in the coatings with depth before - the lower curve and after irradiation - the upper curve (b)

4. CONCLUSIONS

We suggested a mathematical model and implemented the algorithm for computing temperature fields in two-layer metal heat absorbers with a moving irradiation source. On the basis of calculation of temperature fields we recommended certain modes for irradiation of Co-based plasma-detonation coatings by DC pulse plasma jet. The experimental data on the change of structure and phase composition of the coatings and their properties after exposure indirectly confirm the correctness of the calculations of temperature fields.

The mechanism of coating improvement was identified. In general the structure-phase changes are represented by the increase of nanosized intermetallic phase volume concentration and the increase of the width of the diffuse zone in the coating layer contacting the substrate.

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