PROCEEDINGS OF THE INTERNATIONAL CONFERENCE NANOMATERIALS: APPLICATIONS AND PROPERTIES
Vol. **1** No 4, 04PITSE12(3pp) (2012)

Computer Simulation of Temperature Profiles for E-beam Modification of Ni- Based Plasma Detonation Coatings

D.L. Alontseva[1,*], A.L. Krasavin[1], T.A. Kolesnikova[1], A.D. Pogrebnjak[2,†], A.V. Russakova[3,‡]

[1] *East – Kazakhstan State Technical University, 69, Protazanov St., 070004 Ust-Kamenogorsk, Kazakhstan*
[2] *Sumy State University, 2, Rymsky Korsakov St., 40007 Sumy, Ukraine*
[3] *Eurasian National University, 5,Munaitpasov St., 010008 Astana, Kazakhstan*

(Received 16 July 2012; published online 26 August 2012)

The paper presents the calculation of the distribution of the temperature profile in two-layer metallic materials under direct current low-energy electron beam irradiation and proposes explicit parameters of the electron beam for modification of thick (150-300 microns) plasma detonation Ni-based coatings by irradiation. Ni-based coatings deposited onto steel substrates were interpreted as a Ni-Fe two-layer sample irradiated on the coating side. The numerical simulation methods were used for solving the heat equation. The model takes into account the electron beam travelling, dependence of heat conductivity and specific thermal capacity coefficients on the temperature and heat loss for emission from the surface. The design modes were used to carry out the modification by e-beam.

Keywords: Temperature profile, Two-layer metal materials, Electron beam.

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 Ni-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). Based on this model, one can choose the parameters of irradiation so as to develop sufficiently high temperatures on the boundary of the coating to the substrate to accelerate the diffusion processes in order to improve adhesion of the coating to the substrate. The sources devoted to the development of such a model [3,4] testify the relevance of this problem, but they do not provide a comprehensive solution.

The aim of this work is to propose a model of temperature distribution in two-layer metal absorbents during irradiation by a direct current electron beam depending on the energy and beam current density; on the basis of a simulation experiment on the calculation of temperature profiles to recommend specific irradiation modes; to carry out the exposure to radiation according to these modes.

2. EXPERIMENT

The protective coatings with a thickness of 150 to 300 microns were formed on a substrate of quality carbon steel St3 ($20 \times 30 \times 10$ mm^3 samples) using "Impulse-6" plasma-detonation facility. They were deposited with the PG-10N-01 and PG-AN-33 (Russian standards) Ni-based powder alloys.

The irradiation of samples on the side of the surfaces according to the calculated modes was carried out in vacuum by an electron beam on "U-212" generator with an accelerating voltage of 30 kV. The scan is sawlike; the beam travel speed in the horizontal direction is 360 mm/min; the diameter of the electron beam on the sample is 10 mm; the current amperage is 20-30mA.

The need for a detailed explanation of the coating structure scheme stems from the fact that in order to develop a mathematical model of temperature distribution in the coating during irradiation we have to justify the choice of material and thickness of the irradiated layers. Resting on reliable experimental data [5-7] we proposed a layered scheme of the coating structure [8]. A thin layer (less than 5 microns) with mostly Cr oxides and carbides forms on the coating surface. Then comes the main layer of the Ni-based coating, 100-300 microns thick, then a layer of Fe (substrate), 10 000 microns thick. Because of the small thickness of the Cr layer on the surface, this layer was neglected when calculating the temperature profile during electron irradiation, and Ni-Fe double-layer coatings irradiated from the Ni side were considered.

In order to formulate the problem of describing the heating of the coated sample by a moving electron beam as a boundary problem of heat conductivity theory, it is necessary to specify the density of heat sources in a composite solid body. Since the thickness of the coating layer in which the electron beam is almost

* dalontseva@mail.ru
† alex@i.ua
‡ arussakova@gmail.com

completely absorbed is very small compared to the thickness of the coating, and we are interested primarily in the temperature field at the boundary surface between the coating and the substrate, we simulate a moving beam of electrons by a moving flat normal-circular source of a given power, i.e. we assume that the specific heat flux at a distance r from the point of intersection of the symmetry axis of the beam with the sample surface is given by expression (1) (without considering losses):

$$q(r) = q_{max}\exp(-kr^2), \qquad (1)$$

where $q_{max}=kN/\pi$ (N- beam power, $N=U_kI$, where U_k- cathode voltage, and I – the beam amperage), and the heat flux concentration ratio k is correlated with the heating spot radius R_b (the beam radius) by the formula $k=1.125/R_b^2$. The analytical solution of the problem of heating a plate of finite thickness with a moving normal-circular source presented in the literature [9] makes it possible to roughly estimate the maximum heat value of the points on the unheated sample surface. The corresponding calculations for the given ranges of beam energies and the geometrical dimensions of the sample show that the maximum heating (the difference between the maximum temperature reached by a point and the initial temperature of the sample) for the points on the ends and the "back" side of the plate does not exceed 3° C. Thus, the nature of the heat exchange with the environment on the unheated plane of the substrate and the ends of the sample has little effect on the temperature distribution in the contact area of the substrate and coating; and we simulate a sample by an infinite plate of thickness h lying on the surface of the semi-infinite space filled with a material with desired thermal characteristics.

Introducing the Cartesian coordinates by the method indicated in Fig. 1 (X and Y axes lie in the plane of the surface coating, Z axis points into the sample), we believe that at the time $t_0=x_0/v$ a normally circular source begins to operate at the surface, its center moves uniformly with velocity v along the axis X, and switches off at time $t_1=-t_0$ (and at time $t=0$ corresponds to the passage of the beam center point with the coordinates $O(000)$.

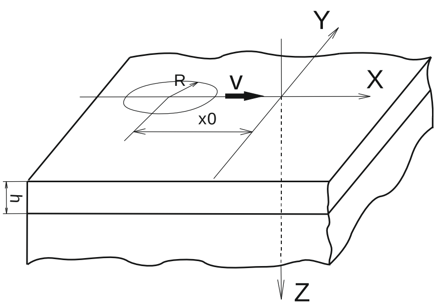

Fig. 1 – Schematic representation of a two-layer sample with a moving spot during heating by the electron beam, indicating the choice of the coordinate system.

Since the heating occurs in vacuum, we believe that the only mechanism of heat loss from the heated surface of the coating is the heat emission described by the Stefan-Boltzmann equation

$$P=\sigma\varepsilon T^4 \qquad (2)$$

where p - beam surface power density [W/m^2] σ - the Stefan-Boltzmann constant, ε – the emissivity factor for the coating material.

Thus, we have the following problem of heat conductivity theory: find function $T_1(x,y,z,t)$ (temperature of the coating) and $T_2(x,y,z,t)$ (substrate temperature), as defined in areas S_1 and S_2 respectively (area S_1 is defined by the inequalities $0 \le z \le h$, $t_0 \le t \le t_1$, while are S_2 is defined by the inequalities $h \le z \le \infty$ and $t_0 \le t \le t_1$, at that for both areas $x \epsilon (-\infty, \infty)$ and $y \epsilon (-\infty, \infty)$), that comply in these areas with the differential equations (3) and (4):

$$\frac{\partial T_1}{\partial t} = \frac{1}{c_1\rho_1}\left[\frac{\partial}{\partial x}\left(\lambda_1\frac{\partial T_1}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_1\frac{\partial T_1}{\partial y}\right) + \frac{\partial}{\partial z}\left(\lambda_1\frac{\partial T_1}{\partial z}\right)\right] \qquad (3)$$

$$\frac{\partial T_2}{\partial t} = \frac{1}{c_2\rho_2}\left[\frac{\partial}{\partial x}\left(\lambda_2\frac{\partial T_2}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda_2\frac{\partial T_2}{\partial y}\right) + \frac{\partial}{\partial z}\left(\lambda_2\frac{\partial T_2}{\partial z}\right)\right] \qquad (4)$$

where $\lambda_1=\lambda_1(T)$ the thermal conductivity of the coating material, considered as a function of temperature and $\lambda_2=\lambda_2(T)$ the thermal conductivity of the substrate material, also considered as a function of temperature. In the calculations for computing the values of the functions $\lambda_1(T)$ and $\lambda_2(T)$ we used polynomal interpolation on tabulated values of thermal conductivity of nickel and iron, $c_1=c_1(T)$ and $c_2=c_2(T)$ – specific heat capacity of the coating and the substrate, respectively, also considered as a function of temperature; ρ_1 and ρ_2 the density of the coating and the substrate materials (the constants), when the initial and boundary conditions described below are met:

the initial conditions: $T_1(x,y,z,t_0)=T_0$ and $T_2(x,y,z,t_0)=T_0$, where T_0 - the initial temperature of the sample set equal to $T_0=20$℃;

the boundary conditions (5), (6) , (7) и (8): at the boundary $z=0$ (the coating surface) –condition (5)

$$k_1\left[(T_1)_P\right] \times \left(\frac{\partial T_1}{\partial z}\right)_P = q_{max}\exp\left(-kr^2\right) - \sigma\varepsilon\left(T_1\right)_P^4, \qquad (5)$$

where $P(x,y,0)$ – the point on the surface of the coating, and $(T_1)_P=T_1(x,y,0)$ and $\left(\frac{\partial T_1}{\partial z}\right)_P$ respectively, the values of the temperature and the normal derivative of temperature at the point P, k_1 – thermal conductivity of the coating material (depending on the temperature), $r=\sqrt{\left(X_ц(t)-x\right)^2+y^2}$ – the distance from point P to the center of the normally circular source $(X_ц(t)=X_0+vt)$;

at the boundary between the coating and the substrate (plane z = h) must be met the two conditions (6) and (7):

$$k_1\left(T_1|_{z=h}\right) \times \frac{\partial T_1}{\partial z}\Big|_{z=h} = k_2\left(T_2|_{z=h}\right) \times \frac{\partial T_2}{\partial z}\Big|_{z=h} \qquad (6)$$

where $k_2 = k_2(T_2)$ the thermal conductivity of the substrate material, considered as a function of temperature

$$T_1(x,y,h) = T_2(x,y,h) \qquad (7)$$

that is, for all x, y and any t, belonging to the interval (t,t_0) at z tending to infinity, the temperature tends to the initial temperature of the sample T_0, condition (8)

$$\lim_{z\to\infty} T_2(x,y,z,t) = T_0 \qquad (8)$$

3. RESULTS

The problem was being solved by the finite-difference method. We used the data [10] for the values of the thermal conductivity, emissivity, specific heat and density of Ni and Fe. Fig. 2 shows the dependence of the temperature at the point with the coordinates *(0,0,h)* (the point that lies at the boundary surface between the coating and the substrate) on the time at the following design parameters: coating thickness h=300 μm, the beam power *N=300W* (cathode voltage U_k=30 kV , beam amperage I=20 mA), beam radius R_b=5 mm, beam velocity v=0.004 m/s, calculation time interval t_1-t_0=14s (t_0=7.0s), correspondingly x_0=-28 mm. Fig. 2b displays the corresponding temperature dependence on the z coordinate for the point with the coordinates x=0, y=0 at the time t=0 at the above calculated parameters (the source switches on at the time t_0=7.0 s, time t=0 corresponds to the center of the source passing the point with the coordinates(0,0,0)).

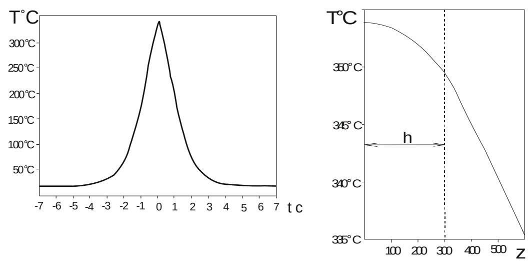

Fig. 2 -Dependence of the temperature of a sample point on the boundary of the substrate and the coating on the time at the surface heating by a moving beam of electrons (a) and the corresponding temperature dependence on the coordinate z (b)

The samples of Ni-based coatings were additionally irradiated according to the modes recommended in the result of numerical simulation calculation: electron beam current density – 20 mA/cm^2, accelerating voltage – 30 kV, in the continuous exposure regime.

For practical calculations at low electron energies we needed to turn to the experimentally obtained patterns. The empirical evidence [11] suggests that the 1-2 mm thick Ni layer at the energies of the electron beam of 30 keV is being completely absorbed. Since the depth of the total absorption of electrons is extremely small in comparison with the thickness of coatings, a model of surface distributed sources of heat can be taken for the construction of the temperature profile in the sample. In our proposed model not only a high temperature in the boundary zone is achieved, but also long enough, the order of several seconds, holding of the area in the high temperature diapason of 400° C is provided, which allows for diffusion processes. The model enabled to choose low current density values, which allows one to save energy for further processing, without penetration into the coating or substrate.

4. CONCLUSIONS

Based on the model of temperature distribution in two-layer absorbents with the surface distribution heat sources, the temperature profiles were calculated according to the irradiation parameters and conditions. The choice of materials and thicknesses of absorbent layers is based on the experimentally developed scheme of the structure of thick plasma-detonation powder coatings. Basing on the calculations we proposed the modes of exposure leading to the formation of high temperatures in the coating - substrate contact zone to accelerate diffusion processes.

REFERENCES

1. K.K. Kadyrzhanov, F.F. Komarov, A.D. Pogrebnyak, V.S. Russakov, T.E. Turkebaev, *Ion-beam and Ion-plasma Modification of Materials* (MGU: Moscow: 2005).
2. E. Celik, I. Ozdemir, E. Avci, Y. Tsunekawa, *Surf. Coat. Tech.* **193**, 297 (2005).
3. G.Z. Ganeev, S.B. Kislitsin, *The calculation of temperature fields, thermal stresses, thermal erosion during pulsed irradiation by an electron flow*, in: Abstract Book of 7th International Conference Nuclear and Radiaion Physics, Almaty, Kazakhsnan, 34 (2009).
4. N.I. Pischasov, A.V. Nikolaev, *Communications of Omsk University* **2**, **3**9 (1996).
5. D.L. Alontseva, S.N. Bratushka, A.A. Borysenko, N.V. Prokhorencova, V.T. Shablya, *Metallofiz. Noveish. Teknol.* **33**, 721 (2011).
6. D. Alontseva, *Przegląd Elektrotechniczny* **86** No7, 42 (2010).
7. A.D. Pogrebnjak, Sh.M. Ruzimov, D.L. Alontseva, *Vacuum* **81**, 1243 (2007).
8. D.L. Alontseva, *Creating the Firm, Wear-Proof and Corrosion-Resistant Coatings on Base Of Ni-Cr and Co–Cr Powder Alloys by Plasma Detonation Method*, in: Abstract Book of the Fourth International Conference "Deformation & Fracture of Materials and Nanomaterials" 446, Moscow, 2011.
9. N.N. Rykalin, *Calculations of thermal processes in welding.*-(Moscow: Mashgiz: 1951).
10. C.I. Smithells, *Metals Reference Book*, (Metallurgiya: 1980).
11. I.A. Abroyan, A.N. Andronov, A.I. Titov, *Physical basis of electronic and ionic technology*, (Higher: 1984).