

# Mathematical Modeling of Temperature Fields in Two-Layer Heat Absorbers for the Development of Robotic Technology for Microplasma Spraying of Biocompatible Coatings

D. L. Alontseva<sup>( $\boxtimes$ )</sup>, A. L. Krasavin, D. M. Nurekenov, and Ye. T. Zhanuzakov

D. Serikbayev East Kazakhstan State Technical University, Ust-Kamenogorsk, Kazakhstan dalontseva@mail.ru, alexanderkrasavin@mail.ru, zhan\_erzhan@mail.ru http://www.ektu.kz

Abstract. The motivation for the research was the challenges faced in developing the robotic microplasma spraying technology for applying coatings from biocompatible materials onto medical implants of complex shape. Our task is to provide microplasmatron movement according to the complex trajectory during the surface treatment by microplasma and to solve the problem of choosing the speed of the microplasmatron movement, so as not to cause melting of the coating. The aim of this work was to elaborate mathematical modeling of temperature fields in two-layer heat absorbers: coating-substrate depending on the velocity of microplasmatron with a constant power density. A mathematical model has been developed for the distribution of temperature in twolayer absorbers when heated by a moving source and the heat equation with nonlinear coefficients has been solved by numerical methods.

**Keywords:** Heat equation  $\cdot$  Two-layer metal heat absorbers  $\cdot$  Computer simulation

## 1 Introduction

The multi-purpose methods of Thermal Coating have recently become popular all over the world [1,2]. One of the major methods of gas-thermal deposition of coatings is plasma spraying. The micro plasma spraying (MPS) method is characterized by a small diameter of a spraying spot  $(1 \dots 8 \text{ mm})$  and low (up to 2 kW) power of plasma, which results in low flow of heat into the substrate [3-5]. These characteristics are very attractive for the deposition of coatings with high accuracy, in particular for applying biocompatible coatings in the manufacture of medical implants.

However, the treatment of surfaces of complex shape can be difficult for the implementation of the thermal spraying technology and requires automated

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manipulations of the plasma source and/or the substrate along with robotic control for appropriate surface treatment [1,2].

At present, robot manipulators are widely used in metallurgical industry, automotive industry and mechanical engineering, allowing automating the plasma processing. However, they are used only for large-scale production, because every transition to a new product requires complex calibration procedures to achieve compliance with the model set in the robot previously. Thus, the problem of automatic code generation of a robot program for the model specified by means of CAD is in the limelight of researchers and developers of robotic systems [6–8].

The main prerequisites for the development of the research were the analysis of technical difficulties arising from the industrial robot exploitation for coating by plasma jets, and the desire to expand the scope of tasks solved by the exploitation of an industrial robot. The authors of this paper have carried out a work in the field of application of automated plasma methods of biocompatible or protective coating deposition, described in our paper [9] and protected by certificates of intellectual property [10,11]. One of the main challenges of the robotic technology of microplasma spraying is the choice of modifying irradiation with a microplasma jet in order to set a certain speed of movement of a robot manipulator with a plasma source along the treated surface. Successful deposition of biocompatible coatings with sustained characteristics on parts of complex shape, which are endoprospheses, requires steady travelling with specified speed and power density of the plasma source along the sprayed surface of the product. In order to choose the desired modes of microplasma surface treatment, we need assumptions about the temperature fields that form during irradiation, because it is the temperature that determines the phase transitions in the coatings. The purpose of this study is to develop a mathematical model for the distribution of temperature fields in two-layer absorbers (coating/substrate) under modifying microplasma irradiation of coatings from biocompatible metals (Titanium or Tantalum).

## 2 Results and Discussion

### 2.1 Brief Description of the Developed Mathematical Model

We have considered the problem of heating a sample, which is a metal plate (substrate) with the deposited on its surface by a moving axisymmetric heat source coating layer (Fig. 1). The choice of material and layer thicknesses of the absorbers were based on the previously developed scheme of the structure of the protective powder coating applied by a plasma jet on the steel substrate described in [12, 13].

The task of heating a plate by a moving flat heat source comes down to the solution of a boundary value problem for a differential equation of heat conductivity. As thermal characteristics of metals, such as thermal conductivity and specific heat, highly depend on temperature, and in processes of radiation treatment of coatings, temperature difference between various points of the sample



**Fig. 1.** Moving flat heat source, where 1-coat; 2-substrate; XYZ - moving Cartesian coordinate system.

can exceed 1000K (flash-off of a surface of the sample at maintaining the temperature of end faces of a plate close to room), adequate mathematical model of thermal processes at radiation treatment of coatings is a non-linear heat conduction equation considering dependence of thermal characteristics of material on temperature.

#### 2.2 Non-linear Heat Conduction Equation. Kirchhoff Transformation

The heat conduction equation for the homogeneous environment whose thermal characteristics depend on temperature in case of lack of sources of heat distributed in the environment, is:

$$div(k(T)\nabla(T)) = c(T)\rho(T)\frac{\partial T}{\partial t}.$$
(1)

In the Eq. (1) T (x, y, z, t) a dynamic field of temperatures taken in an absolute scale (degrees Kelvin), k(T) - function of dependence of a thermal conductivity of substance on temperature, c(T) function of dependence of specific heat of substance on temperature,  $\rho(T)$  - function of dependence of density of substance on temperature. Further on, we will use a differential equation (5) that the Eq. (1) turns into after Kirchhoff transformation [14].

$$\vartheta(x, y, z, t) = \int_{T_0}^{T(x, y, z, t)} k(\tau) d\tau$$
(2)

For the sake of convenience, we believe value of the  $T_0$  parameter equal to environment temperature. As at any moment t temperature T(P,t) in the arbitrariest point P meets condition  $T(P,t) \ge T_0$ , taking into account nonnegativity of the function k(T) we can claim that for display  $T(x, y, z, t) \rightarrow \vartheta(x, y, z, t)$ , set by formula (2) exists the inverse display, i.e. there is a  $T = T(\vartheta)$ .

The remarkable property of Kirchhoff's transformation that

$$\nabla \vartheta = k(T) \cdot \nabla T \tag{3}$$

and, as a result

$$div(k(T) \cdot \nabla T) = \Delta \vartheta \tag{4}$$

Taking into account these identities, the differential equation of heat conductivity (1) turns into a differential equation (5) for function  $\vartheta$ 

$$\Delta \vartheta = Q(\vartheta) \cdot \frac{\partial \vartheta}{\partial t} \tag{5}$$

where

$$Q(\vartheta) = \frac{c(T(\vartheta)) \cdot \rho(T(\vartheta))}{k(T(\vartheta))}$$
(6)

To apply transformation of Kirchhoff to the solution of boundary value problems of the theory of heat conductivity, it is necessary to reformulate the boundary conditions set for function T, in boundary conditions for function  $\vartheta$ . Further on we will believe that the boundary value problem is formulated for the given area of space  $\Omega$ , and a symbol  $\partial\Omega$  will be designated as an area border. Let's consider separately cases of boundary conditions of the 1st and 2nd sort.

(A) The boundary conditions of the 1st sort set by the Eq. (7)

$$\vartheta_{in}(M,t) = \vartheta(T_{in}(M,t)) \tag{7}$$

where  $T_{in}(M, t)$  the function setting distribution of temperatures on area border. As it has been shown above, there is a uniquely determinated function  $\vartheta(T)$ . Let's define on area border  $\Omega$  function  $\vartheta_{in}$ 

$$\vartheta_{in}(M,t) = \vartheta(T_{in}(M,t)) \tag{8}$$

Then a boundary condition (6) for function T(x, y, z, t) will 1 turn into a boundary condition (9) for function  $\vartheta(x, y, z, t)$ .

$$\vartheta_{|\partial\Omega} = \vartheta_{in}(M, t) \tag{9}$$

(B) The boundary conditions of the 2nd sort set by the Eq. (10)

$$-\left(k(T)\cdot\frac{\partial T}{\partial \overrightarrow{n}}\right)_{\partial\Omega} = P(M,t) \tag{10}$$

where function P(M, t) describes the surface density of power of the heat sources affecting the area border. Owing to equality (2), the boundary condition for function  $\vartheta$  looks like (11).

$$-\left(\frac{\partial\vartheta}{\partial\overrightarrow{n}}\right)_{\partial\Omega} = P(M,t) \tag{11}$$

The Eq. (5) in comparison with the Eq. (1) has much simpler structure allowing using well developed potential theory methods for the decision in some cases.

#### 2.3 The Limiting Stationary State When Heating a Plate by Moving a Flat Heat Source. Differential Equation of the Limiting Steady-State

Let's introduce a concept of the limiting steady-state when heating a body by moving heat source. For this purpose we will consider the task given below about heating the semi-infinite body by moving heat source. The obtained results hereafter naturally extend multilayer plates of the terminating sizes

Let axes X and Y of a Cartesian coordinate system lie on the surface of the homogeneous semi-infinite body, with thermal characteristics of k(T), c(T), and density  $\rho(T)$ . Axis Z is sent to the body depth (at such choice of a frame, the semi-infinite body represents area of space set by inequality  $z \ge 0$ ). Let's assume that in an initial instant of t = 0 the flat source of heat moving with constant speed  $\overrightarrow{v} = v \cdot \overrightarrow{i}$ , where v - the speed module, and  $\overrightarrow{i}$  - a coordinate basis vector of collinear axes X begins to act on a surface of sample. Let us assume that the source of heat has an axial symmetry, and in an initial instant axis Z of a Cartesian coordinate system coincides with a source axis. Let us note that the assumption of a axial symmetry of the heat source is insignificant at a conclusion of a differential equation of the limiting steady-state, and it is introduced, first, for simplification, secondly, as the case that is most often found in practice. Let the surface power density of a source be described by the P(r) function where r distance to a source. In that case, a dynamic temperature profile of T(x, y, z, t)in a semi-infinite body will satisfy a differential equation (1) and a regional condition (12) on the sample surface (z=0 plane), the initial conditions (13) and a condition (14)

$$-\left(k(T)\cdot\frac{\partial T}{\partial \overrightarrow{n}}\right)_{z=0} = P(\sqrt{(x-\vartheta\cdot t)^2 + y^2 + z^2})$$
(12)

$$\Gamma(x, y, z, 0) = T_0 \tag{13}$$

$$\forall x, y, t \lim_{z \to \infty} T(x, y, z, t) = T_0 \tag{14}$$

Let us turn into the relative frame Cartesian coordinate system moving with a speed of v, with axes of  $X^*, Y^*, Z^*$  parallel to axes X, Y, Z of the above described fixed frame. Coordinates of a point  $x^*, y^*, z^*$  in a relative frame of logical coordinates are connected with coordinates x, y, z of the same point in the fixed frame (15), (16) and (17).

$$x = x^* + \vartheta \cdot t \tag{15}$$

$$y = y^* \tag{16}$$

$$z = z^* \tag{17}$$

Let  $T^*(x^*, y^*, z^*, t)$  the function describing a temperature field in a relative frame of coordinates. Using differentiation rules and coordinate transformation formulas (15), (16) and (17) we will obtain

$$\frac{\partial T}{\partial x} = \frac{\partial T^*}{\partial x^*} \tag{18}$$

$$\frac{\partial T}{\partial y} = \frac{\partial T^*}{\partial y^*} \tag{19}$$

$$\frac{\partial T}{\partial z} = \frac{\partial T^*}{\partial z^*} \tag{20}$$

$$\frac{\partial T}{\partial t} = \frac{\partial T^*}{\partial t^*} - \vartheta \frac{\partial T^*}{\partial x^*} \tag{21}$$

Thus, the differential equation (1) turns into a differential equation (22) for the function  $T^*$ :

$$\frac{\partial}{\partial x^*} \left(k \cdot \frac{\partial T^*}{\partial x^*}\right) + \frac{\partial}{\partial y^*} \left(k \cdot \frac{\partial T^*}{\partial y^*}\right) + \frac{\partial}{\partial z^*} \left(k \cdot \frac{\partial T^*}{\partial z^*}\right) = c \cdot p \cdot \left(\frac{\partial T^*}{\partial t} - \vartheta \frac{\partial T^*}{\partial x^*}\right) \quad (22)$$

The Eq. (22) can be considered a special case of the equation of Fourier Ostrogradsky for the moving environment [9]:

$$div(k \cdot \nabla T) + q_v = p \cdot c \cdot \frac{DT}{dt}$$
(23)

In the Eq. (23)  $q_v$  - apparent density of sources of heat, and a  $\frac{DT}{dt}$  symbol designates the substantive derivative T determined by a formula (24)

$$\frac{DT}{dt} = \frac{\partial T}{\partial t} + (\nabla T, \vec{v})$$
(24)

It is logical to assume that when the travel time of source is aiming to infinity, in the frame traveling together with a source, the quasistationary temperature profile will be observed, in other words, we can put in the Eq. (23)  $\frac{\partial T^*}{\partial t^*} = 0$ . We will name this mode the limiting steady state, described by differential equation (25).

$$\frac{\partial}{\partial x^*} \left(k \cdot \frac{\partial T^*}{\partial x^*}\right) + \frac{\partial}{\partial y^*} \left(k \cdot \frac{\partial T^*}{\partial y^*}\right) + \frac{\partial}{\partial z^*} \left(k \cdot \frac{\partial T^*}{\partial z^*}\right) + \vartheta \cdot \left(\frac{c \cdot \rho}{k}\right) \cdot \left(k \cdot \left(\frac{\partial T^*}{\partial x^*}\right)\right) = 0 \quad (25)$$

Applying transformation of Kirchhoff to this equation, we will obtain

$$\Delta \vartheta + v \cdot Q(\vartheta) \cdot \frac{\partial \vartheta}{\partial x} = 0 \tag{26}$$

#### 2.4 Heating of Semi-infinite Body by Moving Flat Heat Source

This section is devoted to the description of the numerical method of task solution of heating a half-space by a moving heat source. It should be noted that this task solution allows finding rather precise estimates of a temperature schedule in the field of border of a substrate coating. First of all, we will formulate a boundary value problem for function  $\vartheta(x, y, z)$  representing transformation of Kirchhoff of a temperature field T(x, y, z), in a coordinate system. As it has been shown above, function  $\vartheta(x, y, z)$  o satisfy a differential equation (23) in the  $z \ge 0$ 

$$\nabla\vartheta + v \cdot Q(\vartheta) \cdot \frac{\partial\vartheta}{\partial x} = 0 \tag{27}$$

At boundary conditions (28) and (29):

$$\left(\frac{\partial\vartheta}{\partial z}\right)_{z=0} = -P(x,y) \tag{28}$$

$$\lim_{z \to \infty} \vartheta(x, y, z) = \vartheta_0 \tag{29}$$

If (29) a constant  $\vartheta_0$  - transformation of Kirchhoff of environment temperature  $T_0$ .

This boundary value problem can be reduced to a non-linear integral equation for the numerical solution n which would make it possible to develop the iterative method which enters the group of methods of the fixed point of the squeezing operator finding. As well as in many cases of application of iterative methods, in the case considered by us the choice of an initial approximation influences the speed of calculations. For initial approximation finding, we used a method of a linearization of a differential equation (27). It should be noted that in many cases solution of the linearized equation (27) can serve an appropriate approximation of solutions of initial non-linear equation (27).

For further consideration it is handier to use an invariant form of the equation (27)

$$\Delta \vartheta + \nabla \cdot (F(\vartheta) \cdot \overrightarrow{v}) = 0 \tag{30}$$

where  $F(\vartheta)$  is the antiderivative of the function  $Q(\vartheta)$ 

$$\frac{dF(\vartheta)}{d\vartheta} = Q(\vartheta) \tag{31}$$

Certainly, the  $F(\vartheta)$  function is determined within the arbitraries additive constant. For the sake of convenience we will assume

$$F(\vartheta) = \int_{\vartheta_0}^{\vartheta} Q(\vartheta) d\vartheta \tag{32}$$

To show equivalence of the Eqs. (30) and (27) we will consider expression  $\nabla \cdot (F(\vartheta) \cdot \overrightarrow{v})$  (divergence of a field of vectors  $F(\vartheta) \cdot \overrightarrow{v}$ ):

$$\nabla \cdot (F(\vartheta) \cdot \overrightarrow{v}) = (\nabla F, \overrightarrow{v}) + F \cdot (\nabla \cdot \overrightarrow{v})$$
(33)

as

$$\nabla F(\vartheta) = \frac{dF(\vartheta)}{d\vartheta} \cdot \nabla \vartheta \tag{34}$$

and divergence of a constant field of vectors  $\overrightarrow{v}(x,y,z)=(v,0,0)$  equals to zero,  $\nabla\cdot\overrightarrow{v}=0$ 

$$\nabla \cdot (F(\vartheta) \cdot \overrightarrow{v}) = \frac{dF(\vartheta)}{d\vartheta} \cdot (\nabla \vartheta, \overrightarrow{v})$$
(35)

Whence it follows that taking into account (31) we obtain

$$\nabla \cdot (F(\vartheta) \cdot \overrightarrow{v}) = v \cdot Q(\vartheta) \cdot \frac{\partial \vartheta}{\partial x}$$
(36)

Let's look for a scalar field  $\vartheta$  in the form of superposition of fields  $\varphi$  and  $\eta$ 

$$\vartheta(x, y, z) = \varphi(x, y, z) + \eta(x, y, z)$$
(37)

where a scalar field  $\varphi(x, y, z)$  satisfies the equation of Laplace (38)

$$\Delta \varphi = 0 \tag{38}$$

and the boundary condition (39):

$$\left(\frac{\partial\varphi}{\partial z}\right)_{z=0} = P(x,y) \tag{39}$$

The boundary condition (39) forms the boundary value problem 3 for the Laplace equation (38).

Thus, we obtain the following boundary-value problem for the function  $\eta(x, y, z)$ :

To find function  $\eta(x, y, z)$  defined in a half-space  $z \ge 0$  and satisfying in it a differential equation (40)

$$\Delta \eta = -\nabla \cdot \left( F(\varphi + \eta) \cdot \overrightarrow{v} \right) \tag{40}$$

and boundary condition(41) on border of area:

$$(\frac{\partial\eta}{\partial z})_{z=0} = 0 \tag{41}$$

Below we will show how the boundary value problem given above can be reduced to an integral equation for function  $\eta(x, y, z)$ .

Let's consider the following boundary value problem for a Poisson equation: Let function f(x, y, z) satisfies in field of  $z \ge 0$  a Poisson equation (42):

$$\Delta f = \rho \tag{42}$$

where  $\rho(x, y, z)$  the given function on a border (plane z = 0) boundary condition (43):

$$(\frac{\partial f}{\partial z})_{z=0} = 0 \tag{43}$$

As the solution of this boundary value problem serves function (44)

$$f(x,y,z) = \int \int \int G(x',y',z',x,y,z) \cdot \rho(x',y',z') \cdot dx' dy' dz'$$
(44)

Where G(x', y', z', x, y, z) the Green function of this boundary value problem determined by formulas (44) and (45)

$$G(x',y',z',x,y,z) = \frac{1}{4\cdot\pi} \cdot \left(\frac{1}{r(x',y',z',x,y,z)} + \frac{1}{r(x',y',z',x,y,-z)}\right) \quad (45)$$

$$r(x', y', z', x, y, z) = \sqrt{(x - x')^2 + (y - y')^2 + (z - z')^2}$$
(46)

Note: If we use physical interpretation of a Poisson equation in which function f(x, y, z) describes a stationary temperature field, and the function  $\rho(x, y, z)$  is related to the heat density distribution function p(x, y, z) the ratio and the coefficient of thermal conductivity of the environment  $\lambda$  by the relation (47),

$$\rho(x, y, z) = \frac{1}{\lambda} \cdot \rho(x, y, z) \tag{47}$$

Then a design of a Green's function of the above described boundary value problem can be considered as natural generalization of a method of images.

Thus, the boundary value problem (1) for a differential equation (47) comes down to a non-linear integral equation

$$\eta(x,y,z) = -\int \int \int (\nabla \cdot (F(\eta + \varphi) \cdot \overrightarrow{v})) \cdot G(x',y',z',x,y,z) dx' dy' dz' \quad (48)$$

In the last equation the nabla operator represents a symbolic vector

$$\nabla = \left(\frac{\partial}{\partial x'}, \frac{\partial}{\partial y'}, \frac{\partial}{\partial z'}\right) \tag{49}$$

And the factor  $\nabla \cdot (F(\eta + \varphi) \cdot \overrightarrow{v})$  in expanded form registers as

$$\nabla \cdot \left( F(\eta(x', y', z') + \varphi(x', y', z')) \cdot \overrightarrow{v} \right)$$
(50)

Further we suppose that there is a rectangular parallelepiped  $\Omega$ , (defined as  $M(x, y, z) \ni \Omega$  if  $x_{max} \ge x \ge -x_{max}, y_{max} \ge y \ge -y_{max}$  and  $0 \ge z \ge z_{max}$ , such, that  $F \cdot (\eta(x, y, z) + \varphi(x, y, z)) = 0$  at any point A(x, y, z) lying outside this area.

Let's transform a right member of the Eq. (48), integrating piecemeal

$$\left(\nabla \cdot \left(F(\eta + \varphi) \cdot \overrightarrow{v}\right)\right) \cdot G = \nabla \cdot \left(\left(F(\eta + \varphi) \cdot G\right)\right) \cdot \overrightarrow{v} - F(\eta + \varphi) \cdot \left(\nabla G, \overrightarrow{v}\right)\right)$$
(51)

According to the theorem of Gauss - Ostrogradsky

$$\int \int \int_{\Omega} \nabla \cdot ((F(\eta + \varphi) \cdot G) \cdot \overrightarrow{v}) dx' dy' dz' = \int \int_{D} F(\eta + \varphi) \cdot G \cdot (\overrightarrow{n}, \overrightarrow{v}) dS$$
(52)

where  $\overrightarrow{n}$  - a vector of a normal to a surface of border D of the area  $\Omega$ .

On the plane z = 0 vector  $\vec{n} = (0, 0, 1)$  is orthogonal to  $\vec{v}$  vector, i.e., on sides of a parallelepiped D not lying in the plane z = 0  $F(\eta + \varphi) = 0$ .

Thus,

$$\int \int \int_{\Omega} \nabla \cdot \left( (F(\eta + \varphi) \cdot G) \cdot \overrightarrow{v}) dx' dy' dz' = 0$$
(53)

and taking into account (50) we obtain

$$\eta(x, y, z) = \int \int \int_{\Omega} F(\eta + \varphi) \cdot (\nabla G, \overrightarrow{v}) dx' dy' dz'$$
(54)

The problem of finding the solution of a non-linear integral equation (54) can be interpreted as a problem of finding the fixed point of display  $f(x, y, z) \rightarrow Kf(x, y, z)$ , where action of the non-linear operator K is defined by expression (55)

$$Kf(x,y,z) = \int \int \int_{\Omega} F(\eta(x',y',z') + \varphi(x',y',z')) \cdot (\nabla G, \overrightarrow{v}) dx' dy' dz'$$
(55)

We make a hypothesis, that display (55) is the squeezing display, i.e. we assume that there is a constant d < 1, such that  $\forall f_1, f_2 \in U$  is carried out inequality:

$$\|Kf_1 - Kf_2\| < d \cdot \|f_1 - f_2\|$$
(56)

At the same time we designate a symbol U metric space of the square integrable functions defined in the area  $\Omega$ , with a reference metrics:

$$\|f\| = \int \int \int_{\Omega} f^2 dx dy dz \tag{57}$$

It is known that for the squeezing operator K, the repetitive process determined by the equations looks like (58)

$$f_k = K f_{k-1} \tag{58}$$

meets to the fixed point of operator K at any initial approximation of  $f_0$ .

### 3 Conclusion

A mathematical model for the distribution of temperature fields in two-layer absorbers with modifying microplasma irradiation of metallic coatings has been developed and the numerical method for calculating temperature fields in the coating/substrate's system heating by a moving heat source has been designed. Kirchhoff's transformation was applied when solving a nonlinear heat equation by numerical methods. Based on the calculations of the temperature fields, certain speeds of movement of the robot arm with a microplasma source and certain power densities of the plasma source, i.e., microplasma surface treatment modes were recommended in order to ensure the desired temperature distribution in the coating/substrate's system. Coatings from biocompatible materials deposited by the microplasma according to recommended modes onto steel and titanium substrates have been obtained. It is shown that the robotic microplasma spraying method allows applying a wide range of biocompatible materials: Co-based powders, Titanium or Tantalum wires onto medical implants. Thus, the applied value of the developed mathematical model and numerical methods for solving problems of robotic microplasma spraying of biocompatible coatings on endoprostheses has been shown. The results of the research are of significance for a wide range of researchers developing numerical methods for solving nonlinear equations.

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