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PHYSICAL AND MATHEMATICAL SIMULATION OF HEAT AND MASS-TRANSFER IN MICRO-PLASMA AND SPARK PROCESSES WITH VARIOUS AMBIENCE

Alexander A. Kouleshoff[1], Vladislav V. Nelayev[2] and Natalia M. Chigrinova[3]

[1]Equations of Mathematical Physics Department, Belarusian State University F. Skorina av. 4, 220050, Minsk, Belarus

[2]Micro– and Nanoelectronics Department, Belarusian State University of Informatics and Radioelectronics, P. Brovky str. 6, 220600, Minsk, Belarus

[3]Powder Metallurgy Institute of Belarusian National Academy of Sciences B. Platonov str. 12b, 220005, Minsk, Belarus

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Abstract. This work is devoted to physical and mathematical simulation of micro-plasma and spark processes in conditions of various ambiences. Here we present results illustrated possibilities of developed mathematical approach (in the frame of response surface methodology) for description and optimization of advanced materials covering technology, in particularly growth of oxide-ceramic films. Physical modeling of the process with taking into account main mechanisms is a subject of further studies.

1. INTRODUCTION

Joined micro–plasma, electrical discharge, spark, and ultrasound treatments have steadily gained importance over the last years because of their ability to cut and shape a wide variety of solid materials. Advanced materials, such as ceramics, oxides, composites and others, which are difficult to cover by conventional means, have been successfully covered in the Powder Metallurgy Institute of Belarusian National Academy of Sciences [1]. Modeling and simulation of physical mechanisms of separated phenomena of that complex process is the alone way for goal–directed searching of optimal conditions and parameters of qualitative covering and shaping. The main elements of investigated process are two electrodes, a cathode and anode, separated by dielectric, in particularly by liquid dielectric. Physical phenomena in the space between cathode and anode are the object for construction of physical models and following simulation. Simple cathode erosion model for electrical discharge covering was presented in [2]. The heat transfer equation (without heat generation) in the partial differential form was used for description of that phenomenon. The main conclusion of this model – the high density of the liquid dielectric causes plasmas of higher energy intensity and pressure than those for gas discharges.

The physical model proposed in [3] was devoted to erosion of anode material. That model correctly describes rapid melting of an anodic material as well as the subsequent resolidification of the material for long durations of time. Besides, it was explained the low anode erosion rates that result due to resolidification of the anodic piece for long on–times. The base equation for this anode erosion model is the same unsteady–state heat conduction law. The joined theoretical model for description of dielectrical discharge in a liquid media was

Corresponding author: Alexander A. Kouleshoff, e-mail: kuleshov@bsu.by

presented in [4]. Numerical solution of the three differential equations (liquid dynamics, energy balance and radiation) combined with a plasma equation of the state provides plasma radius, temperature, pressure, and mass as a function of pulse time for fixed current, electrode gap and power fraction remaining in the plasma.

However all above models (in spite of their physical transparency) is impossible to use for many–factorial optimization because of complexity of their numerical realization. Here we propose the alternatively mean for the solution of that task using Response Surface Methodology (RSM) well–tried in the same problems of microelectronics [5-10].

2. STATEMENT OF THE PROBLEM

In common case, the boundary problem of the physical simulation micro–plasma and spark processes for covering at galvano–statics mode (GSM) may be written in the following form of the thermal conduction equation:

$$\frac{\partial U}{\partial t} - a \cdot \frac{\partial^2 U}{\partial x^2} - b \cdot \frac{\partial U}{\partial x} - c \cdot U = F(t, x), \quad (1)$$

$$U(0, x) = f(x), \quad (2)$$

$$\frac{\partial U}{\partial x}(0, t) - k_1 \cdot U(0, t) = u_1(x, k_1), \quad (3)$$

$$\frac{\partial U}{\partial x}(L, t) - k_2 \cdot U(L, t) = u_2(x, k_2), \quad (4)$$

where unknown parameters in functions $u_1(x, k_1)$ and $u_2(x, k_2)$ are k_1 and k_2.

Here *U* is the generalized function. In our task *U* is thickness of covering formed in micro–plasma and spark process. In the particular statement such problem was considered in works [2-4]. The boundary conditions must be executed in the coordinate where the current takes extreme values: minimum value under $x=0$ and maximum value under $x=L$.

Under the further solution of the considered problem in RSM–approach, we consider that used mathematical model of the MPS process in the form of the boundary problem of the thermal conduction equation must not take into account detailed mechanisms in accustomed 3–dimensional space. All potential of the mathematical model is enclosed in coefficients *a*, *b*, *c*, k_1, k_2 and in the right parts of conditions (1) – (4), i.e. task data. These data can be restored from the results of the full factorial experiment when we will solve the problem by RSM–methodology.

In the case (without damage for correctness of the further discourses), we can rest on any existing physical interpretation of the problem (1)–(4). Usually it is the problem of the thermal conductivity in the peg with constant section *S* and length *L*. In formula (3) and (4) u_1 are the specified distribution of the value “thickness of the covering” at the left part of the peg Ξ_{left} at the initial time (exactly, under current, equal zero), u_2 is the corresponding value of “thickness of the covering” at the right part of the peg subset Ξ_{right} under the maximum value of the current.

The problem was solved in the system *Mathematica* [11] using RSM–methodology [5].

3. RSM APPROXIMATION OF EXPERIMENTAL DATA AND THEIR SMOOTHING FOR OXIDE–CERAMICS COVERING BY MICRO–PLASMA METHODOLOGY

The initial experimental data are presented below. They are used for construction of approximated polynomial dependencies “thickness of the covering vs technology parameters” needed for optimization procedure by means of RSM approaching [5]. The first variable is time and the last variable is thickness of the covering.

$$data = \{\{10,5,0\},\{10,10,0\},\{10,20,2\},\{10,30,4\},\{10,40,8\},\{20,5,3\},\{20,10,4\},\{20,20,8\},\{20,30,10\},\{20,40,18\},\{30,5,7\},\{30,10,9\},\{30,20,12\},\{30,20,12\},\{30,30,16\},\{30,40,26\},\{40,5,12\},\{40,10,15\},\{40,20,21\},\{40,30,27\},\{40,40,39\},\{50,5,19\},\{50,10,23\},\{50,20,27\},\{50,30,34\},\{50,40,47\},\{60,5,24\},\{60,10,27\},\{60,20,34\},\{60,30,35\},\{60,40,58\},\{70,5,27\},\{70,10,31\},\{70,20,39\},\{70,30,35\},\{70,40,66\}\},$$

The initial data in this problem are specified in the manner of table of the full factorial experiment:

TableForm[data, TableHeadings → {Automatic, {“Time”, “Current”, “CurrentThickness”}}]

Unknown coefficients and right parts of the problem (1) – (4) are determined on the base of above

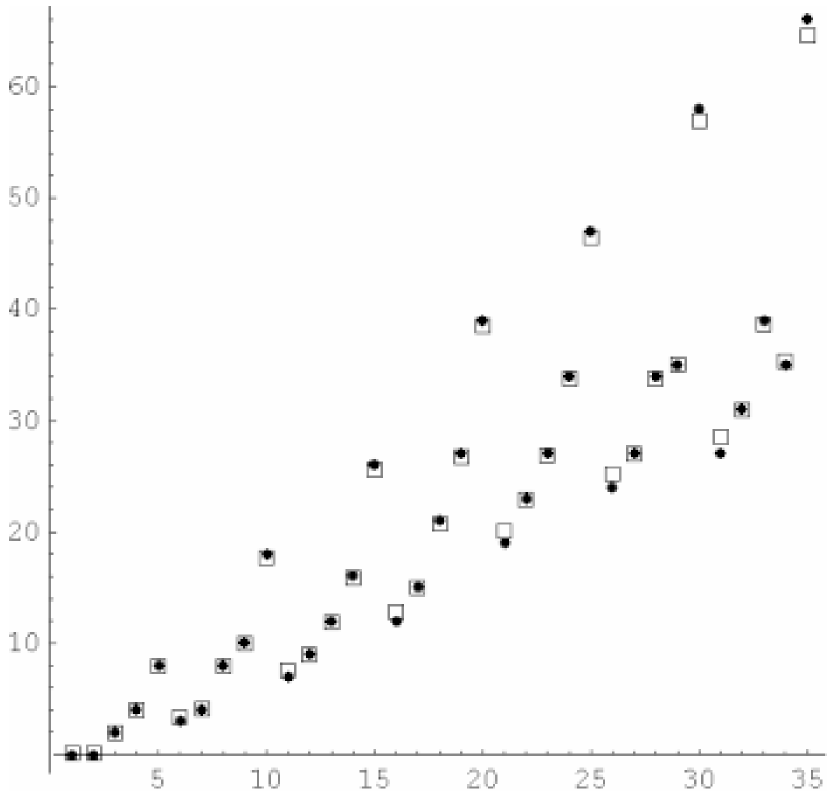

Fig. 1. Initial and smoothing data with the smoothing parameter *a*=0.95. The number of experiment is remitted on the abscissa axis, the covering thickness is remitted on the ordinate axis.

prior information. We are interested in classical solution of that problem, i.e. the function limited in the rectangle Π= [0, 70] ×[0, 40]. It is obviously that the solution *u*(*t*, *x*) have specified values at points of the factorial design, i. e.

$$u(t_i, x_i) = CoveringThickness_i, \quad i = 1,\ldots,35, \qquad (5)$$

or are differed from values *CoveringThickness* on certain value ε since values *CoveringtThickness* can be specified with mistakes.

Selective values of thicknesses must be subjected to exponential smoothing [9] before construction of approximated RSM polynomials “thickness of the covering *vs* technology parameters”. The exponential smoothing is used if there is a serious basis to suppose that experimental results contain mistakes. Results presented in Fig. 1 demonstrate exponential smoothing of “thickness of the covering vs technology parameters” data with the smoothing parameter *a*=0.95.

Initial data in Fig. 1 are shown by filled circles; smoothing data are shown by empty squares. Reduction of the smoothing parameter leads to a serious qualitative changes. For instance, if the parameter of the smoothing *a*=0.1, we get qualitative new result (see Fig. 2). We use the smoothing parameter *a*=0.95 in our next analysis.

Polynomial approximation of experimental results leads to the following expression:

$$\begin{aligned} u(t,x) = {} & 3{,}73901\times10^{-8}\cdot t^3\cdot(-39{,}9362+x)\cdot \\ & (-22{,}9101+x)\cdot(-10{,}7968+x)\cdot \\ & (-8{,}03983+x)+0{,}0000475711\cdot t\cdot \\ & (-38{,}9038+x)\cdot(-24{,}5179+x)\cdot \\ & (-9{,}32304+x)\cdot(-7{,}92575+x)- \\ & 2{,}19672\times10^{-6}\cdot t^2\cdot(-40{,}0911+x)\cdot \\ & (-21{,}3209+x)\cdot(-13{,}9848+x)\cdot \\ & (-5{,}92813+x)-2{,}0069\times10^{-10}\cdot t^4\cdot \\ & (-39{,}725+x)\cdot(-24{,}3399+x)\cdot \\ & (-92{,}7284-18{,}2218\cdot x+x^2)- \\ & 0{,}000271198\cdot(-39{,}9137+x)\cdot \\ & (-23{,}5958+x)\cdot(-74{,}8014-16{,}2236\cdot x+x^2). \end{aligned} \qquad (6)$$

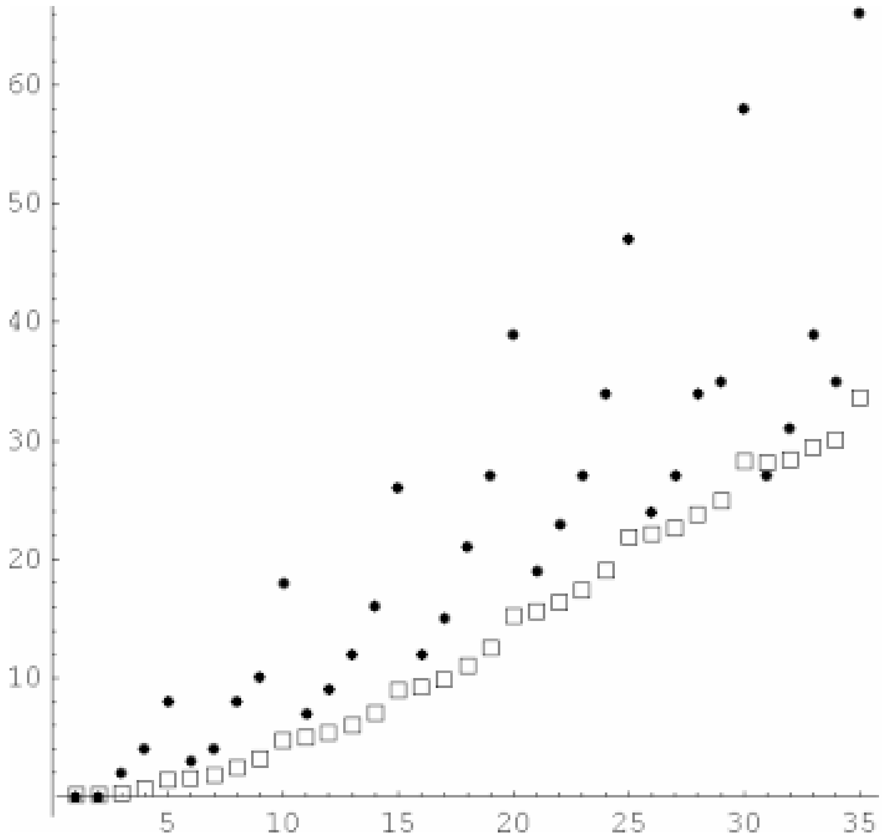

Fig. 2. Initial and smoothing data with the smoothing parameter *a*=0.1 (indications are same as in Fig. 1)

Relative errors of approximation in points of the factorial plan of this regression (in percent):

$$\{\infty, \infty, 7{,}45381, 6{,}83369, 1{,}48975, 1{,}20025, 6{,}43279, 8{,}44327, 11{,}2485, 3{,}43658, 1{,}22464, 1{,}33049, 9{,}85736, 9{,}93996, 5{,}02718, 2{,}96276, 3{,}58005, 4{,}44205, 1{,}79047, 3{,}65149, 2{,}35893, 4{,}01792, 0{,}788032, 2{,}53594, 1{,}77196, 1{,}05187, 2{,}1355, 0{,}317629, 2{,}364, 0{,}415693, 0{,}198862, 0{,}422101, 0{,}128772, 0{,}620796, 0{,}0372904\}. \quad (7)$$

Correlation dependencies (correlation between experimental results and calculated from polynomial $u(t, x)$) are presented in Fig. 3. The points in Fig. 3 are pairs of values “calculation–experiment”, and the line corresponds to linear regression. The results presented in Fig. 3 confirm the goodness between approximations and experimental data.

4. EXTRACTION OF COEFFICIENTS IN EQUATIONS (1) – (4) ON THE BASE OF POLYNOMIAL REGRESSION

From the theoretical standpoint, most interest is the regression, built with use of non–parametric estimation of the conditional mathematical expectation of specified value of the covering thickness with taking into account extreme points of the plan matrix (see Fig. 3) since maximum and minimum values of the solutions of equations (1) – (2) are reached at the boundary of the rectangle ? (in the correspondence with the principle of the maximum value for parabolic equations).

Let’s the solution of equations (1) – (4) is the polynomial regression $u(t,x)$ shown in Fig. 4.

Unknown coefficients and right parts of problem (1) – (4) are determined with use the approximated function $u(t, x)$.

Let the “current conductivity” coefficient be

$$a(t,x) = \frac{\partial u}{\partial t} \Big/ \frac{\partial^2 u}{\partial x^2} \quad (8)$$

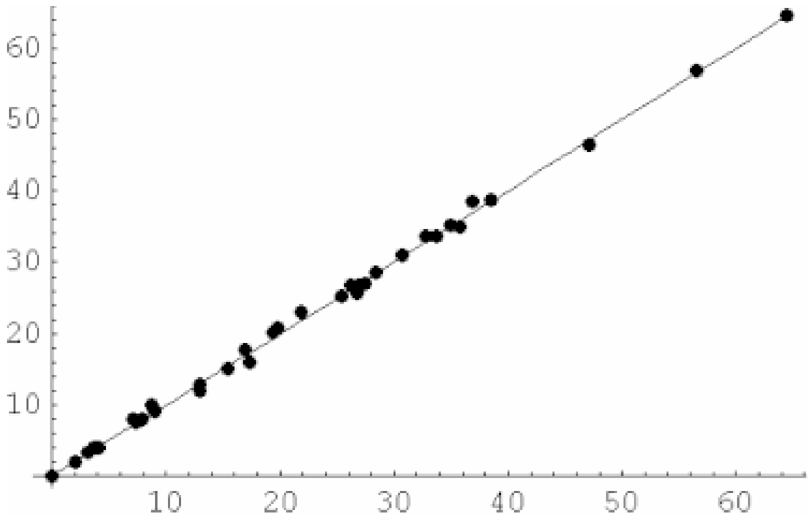

Fig. 3. Correlation dependencies “calculation–experiment”.

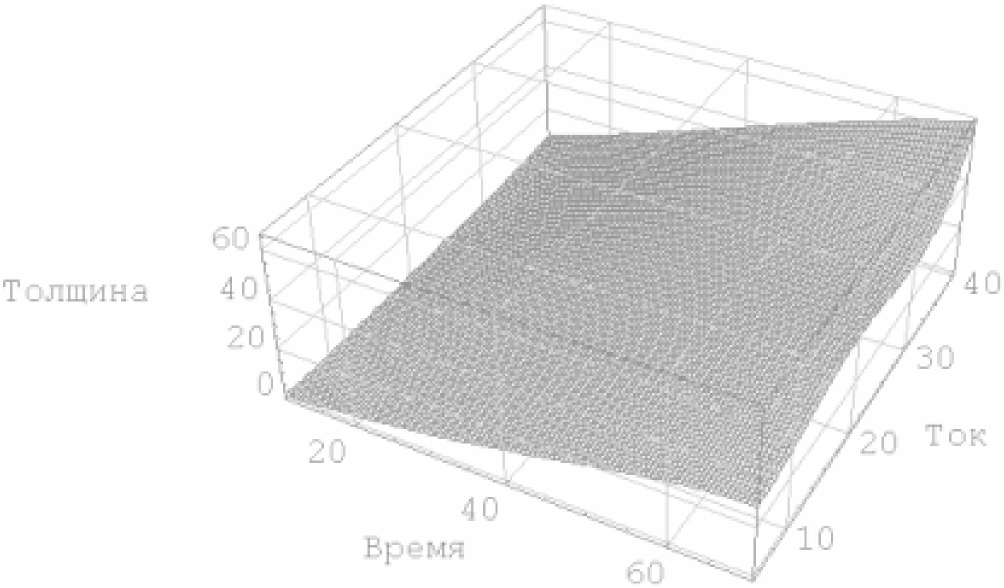

Fig. 4. Dependency “the thickness of oxide–ceramics covering *vs* technology parameters – time and current” for micro–plasma–spark process.

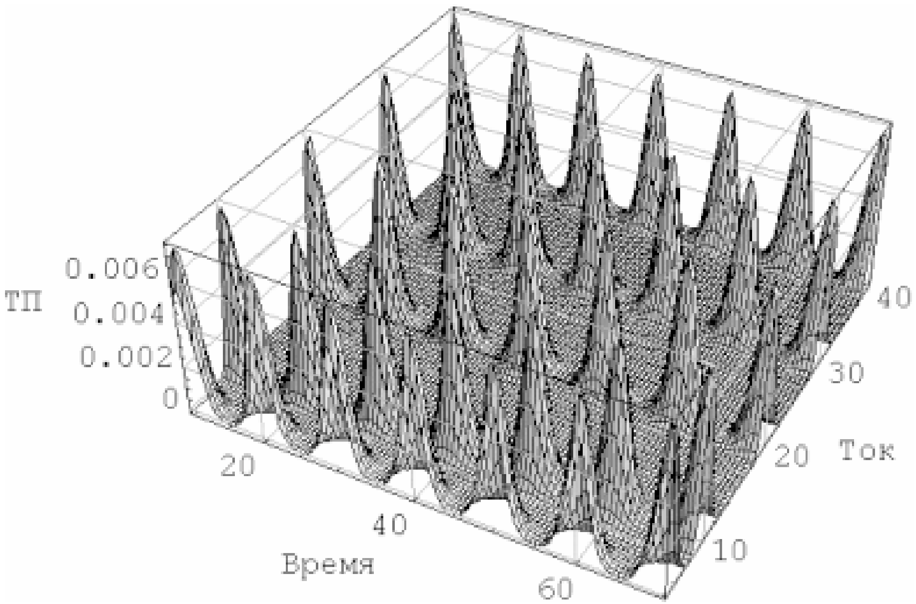

Fig. 5. Distribution density of points (Π) for full factorial design from technology parameters: Time and Current.

Then function $u(t, x)$ will satisfy to the equation

$$\frac{\partial u}{\partial t} - a(t,x) \cdot \frac{\partial^2 u}{\partial x^2} = 0. \quad (9)$$

Determined „current conductivity" coefficient $a(t,x)$ can take and negative values. In order to write Eq. (1) with positive value of „current conductivity" we shall take the series of the agreements.

Let's $K(t, x)$ is the joint distribution density of selective pairs $\{t,x\}$ random quantities {time, current}, found as a result of preliminary experiment. Their number always is certainly:

$$\{t_1, x_1\}, \{t_2, x_2\}, \ldots, \{t_m, x_m\}. \quad (10)$$

Density $K(t, x)$ is restored on the base of sample (10) by means of non-parametric estimation methodology. Density distribution of full factorial design points is shown in Fig. 5.

5. CONCLUSIONS

The problem of physical and mathematical simulation of micro-plasma and spark processes with various ambiences is stated. Strict and economical decision of the optimization of process technological parameters is possible only by use of the response surface methodology. Goal-directed searching for the most significant parameters of investigated technology can be realized on the base of the detail simulation of separate physical mechanisms of micro-plasma and spark process for covering of advanced materials. Here main results of the first part of studies are presented. Physical modeling of the process with taking into account main mechanisms is a subject of the further studies.

Modified algorithm for calculation of the covering thickness with use RSM approximation was described. Standard problem of statistical analysis of experimental data was investigated for technology of oxide-ceramics covering by means of micro-plasma and spark process. Reverse optimization task was solved for determination of micro-plasma and spark technology parameters from the viewpoint of different permissible intervals of oxide-ceramics covering thickness. New computing procedures were proposed for the solution of reverse task in the form of 1-dimensional parabolic equation. Coefficients and boundary conditions were determined for mixed problem simulated by 1-dimensional parabolic equation for description of oxide-ceramic covering technology. Many-dimensional dependencies "thickness of covering vs technology parameters" were calculated and analyzed for conditions of micro-plasma and spark process.

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