The Mathematical Modeling and Computer Simulation of Pulse Electrochemical Micromachining

J. Kozak, D. Gulbinowicz, and Z. Gulbinowicz

Abstract—**The need for complex and accurate three dimensional (3-D) microcomponents is increasing rapidly for many industrial and consumer products. Electrochemical machining process (ECM) has the potential of generating desired crack-free and stress-free surfaces of microcomponents. This paper reports a study of pulse electrochemical micromachining (PECMM) using ultrashort (nanoseconds) pulses for generating complex 3-D microstructures of high accuracy. A mathematical model of the microshaping process with taking into consideration unsteady phenomena in electrical double layer has been developed. The software for computer simulation of PECMM has been developed and the effects of machining parameters on anodic localization and final shape of machined surface are presented.**

Index Terms—**double layer, electrochemical micromachining, ultrashort pulses, mathematical model.**

I. Introduction

The need for complex and accurate three dimensional (3-D) microcomponents is increasing rapidly for many industrial and consumer products. Besides traditional machining techniques such as micro turning and milling, attention is being focused on non-traditional machining techniques such as micro electrical discharge machining (EDM) and micro electro chemical machining (ECMM) and laser machining because of their unique characteristics. Electrochemical machining (ECM) is based on controlled anodic dissolution process of the workpiece (anode) with the tool as the cathode in an electrolyte cell. The ability of ECM in rapidly generating a stress-free and crack-free smooth surface on any electrically conductive material (irrespective of hardness) makes it an excellent choice as a microproduction process.

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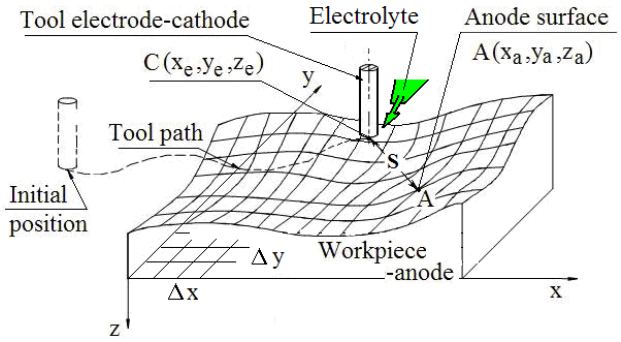


Fig .1: Scheme of Pulse Electrochemical MicroMachining PECMM

Microshape of element is achieved by controlled movement of tool electrode along specified path (Fig. 1). However during ECM material is removed also from zone which is far away from tool electrode due to stray current. It is particularly important in micromachining, because dimension of this zone may be larger than the dimension of produced microstructure. Increase of the localization of electrochemical dissolution (stop dissolution on surface not under tool electrode) is an important problem in EC micromachining with tool electrode, especially an universal tool electrode.

This problem was solved successfully by researchers from Max-Planck Institute in Berlin by using ultrashort pulses with pulse on-time below 200 ns [1]-[3]. It was found that main factor determining the localization of electrochemical dissolution is phenomenon connected with charging the electrical double layer. They showed possibility of geometrical nanostructure fabrication with picoseconds pulses [3]. These articles became an essential incentive for PECMM development in many research institutes in Germany, Korea, Russia, Singapore, US and Poland [4]-[9].

II. Mathematical Modeling and Computer Simulation

The purpose of PECMM process modeling and computer simulation is to determine the final shape of workpiece for a given set of following conditions: initial shape of workpiece described by $z = Z_0(x, y)$; shape and dimensions of the tool electrode, starting position of tool electrode relatively to the workpiece ($x_e^{(0)}, y_e^{(0)}, z_e^{(0)}$); the trajectory and kinematics of the tool electrode: $x_e(t)$, $y_e(t)$ $z_e(t)$; electrical parameters such as working voltage U; electrolyte properties, such as electrical conductivity κ; electrochemical properties of the material of

workpiece described by electrochemical machinability, $K_V = K_V(i)$ (where i is current density);

To formulate the mathematical model, a general case describing change in shape of the surface of the workpiece can be examined using coordinate system attached to the workpiece, which is immovable during machining (Fig. 1 and 2).

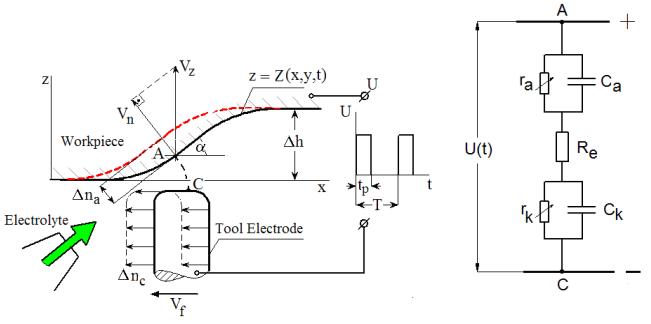


Fig. 2: Scheme for modeling PECMM process

According to electrochemical shaping theory, the evolution of the shape of the workpiece $Z\ (x, y, t)$, can be described as [3, 9]:

$$\frac{\partial Z}{\partial t} = K_v(i_a) i_a \sqrt{1+\left(\frac{\partial Z}{\partial x}\right)^2 + \left(\frac{\partial Z}{\partial y}\right)^2} \qquad (1)$$

where:

$K_V = K_V(i_a)$ - coefficient of electrochemical machinability which is defined as the volume of material dissolved per unit electric charge and for PECMM, the value of K_V is averaged in pulse period, i_a – average current density on the surface of anode during pulse period.

At the beginning of machining: $t = 0$, $z = Z_0(x, y)$, where $Z_0(x, y)$ describes the initial shape of the workpiece surface.

The governing partial differential equations have been solved by the finite difference method for simulating the shape generation by PECMM.

The crucial problem in PECMM is determination of current and electrical charge density during pulse period.

As it is known from electrochemistry, after applying voltage pulse to electrodes, transformation of electron metal conduction into ion electrolyte solution conduction in electrical double layer is realized by two ways: progress of the electrochemical reaction i_f (flow of the Faraday current) and flow of current i_c (the capacity charging current) through a capacitor which is equivalent the electrical double layer on boundary metal – electrolyte solution.

This is a reason that in analysis of electrode process, physical model of the interelectrode space is used in form of electrical circuit shown in Fig. 2.

Capacitance C characterizes the electrical double layer, resistance r – passage of charge through boundary metal – electrolyte and resistance r is called Faraday resistance. In pulse process value of resistance r changes with time and is calculated as $r = \frac{d\varphi}{di}$ where φ is potential. Faraday current intensity is proportional to rate of electrode reaction. For anode this current defines rate of mass exchange therefore rate of workpiece dissolution. This current is dependent on potential difference which is forming close to the electrode surface and is described by Butler – Volmer equation.

The following assumptions have been made in developing a mathematical model of the PECMM process with a tool electrode system shown in Fig. 2 and using nanosecond pulses:

- electrolyte conductivity is constant during pulse,
- adsorption and forming of oxides on electrode surfaces are neglected,
- pulse generator's characteristic is „rigid"; it means that voltage variations as a result of load are omitted,
- influence of geometric nanostructure on electrical field distribution is neglected,
- workpiece material structure heterogeneity is neglected,
- transport of charge through boundary metal – electrolyte is conditioned by electrode process kinetics that is ionization process $Me \rightarrow Me^{ne} + ne$ on anode and discharge cations on cathode.

Because of free charge localized in the double layer area, electrical field in the interelectrode gap is described by Poisson equation. Taking into account fact, that double layer thickness is significantly smaller than the gap size S ($\delta_{DL} \cong 0.4 - 4\ nm \ << \ S\ (\bar{S} > 1000\ nm)$) electrode potentials φ_a and φ_k can be introduced into boundary conditions and the double layer thickness is neglected. Then electrical field distribution in the interelectrode gap is described by Laplace's equation:

$$\nabla^2 u = 0 \qquad (2)$$

with boundary conditions:

on anode $u = U - \varphi_a$ (3)

on cathode $u = \varphi_k$ (4)

on isolated surfaces $z = G_{iz}$ $\left.\frac{\partial u}{\partial n}\right|_{Giz} = 0$ (5)

Potentials φ_a and φ_k on boundary anode – electrolyte and cathode – electrolyte are dependant on current density.

From current balance on the outer Helmholtz plate (on the outer plate of double layers on anode and cathode) it is:

$$\kappa \cdot \left.\frac{du}{dn}\right|_A = C_a \cdot \frac{d\varphi_a}{dt} + i_{fa} \qquad (6)$$

$$\kappa \cdot \left.\frac{du}{dn}\right|_C = C_k \cdot \frac{d\varphi_k}{dt} + i_{fk} \qquad (7)$$

where:

i_{fa}, i_{fk} - Faraday currents on anode and cathode

Faraday currents in accordance with Butler – Volmer equation, appropriately for anode and cathode, are:

$$i_{fa} = i_{0a}\left(\exp[\frac{(1-\alpha)nF\varphi_a}{R\theta}] - \exp[\frac{-\alpha nF\varphi_a}{R\theta}]\right) \qquad (8)$$

$$i_{fk} = i_{0k}\left(\exp[\frac{(1-\alpha)nF\varphi_k}{R\theta}] - \exp[\frac{-\alpha nF\varphi_k}{R\theta}]\right) \qquad (9)$$

where: α - transfer coefficient, n - number of electrons in electrochemical reaction, F - Faraday constant, φ - electrical potential, R - gas constant, θ - temperature, i_0 - exchange current density.

In the mathematical model it is assumed that value of transfer coefficient $\alpha = 0.5$. It is appropriate for the most of workpiece materials. For solving this system of equations, the method of linearization of potential distribution along gap

size S was applied. After transformation the system of equations which describes electrical field parameters are:

$$R_e \cdot (C_a \cdot \frac{d\varphi_a}{dt} + 2 \cdot i_{0a} \sinh\left(\frac{Fn\varphi_a}{2R\theta}\right)) + \varphi_a + \varphi_k = U \quad (10)$$

$$C_a \cdot \frac{d\varphi_a}{dt} + 2 \cdot i_{0a} \sinh\left(\frac{Fn\varphi_a}{2R\theta}\right) = = C_k \cdot \frac{d\varphi_k}{dt} + 2 \cdot i_{0k} \sinh\left(\frac{Fn\varphi_k}{2R\theta}\right) \quad (11)$$

where $R_e = \frac{S}{\kappa}$

with initial conditions for the single pulse with full discharge of double layer after previous pulse

for $t = 0$ $\varphi_a = 0$, $\varphi_k = 0$

In case of pulse series without full gap relaxation, initial condition for pulse j +1 is:

$$\varphi_{a,k}^{j+1}(0) = \varphi_{a,k}^{j}(T) \quad (12)$$

Change of workpiece shape is determinate by distribution of removed material thickness during tool electrode passes. During the period T the thickness of the electrochemically-removed layer at point A on the anode is

$$\Delta n_a = K_v q \quad (13)$$

where q is density of electrical charge transported during pulse period T.

In order to evaluate a quantity of removed material in single pulse and finally changes in anode shape it is necessary to calculate charge q, which flows through a unit surface of anode during single pulse. Therefore, the main goal of a mathematical modeling is a calculation of electrical charge q, and current density $\bar{i}_a$, so after finding a solution $\varphi_a = \varphi_a(t)$, i_{fa}, the values of q and $\bar{i}_a$ are calculated from equations:

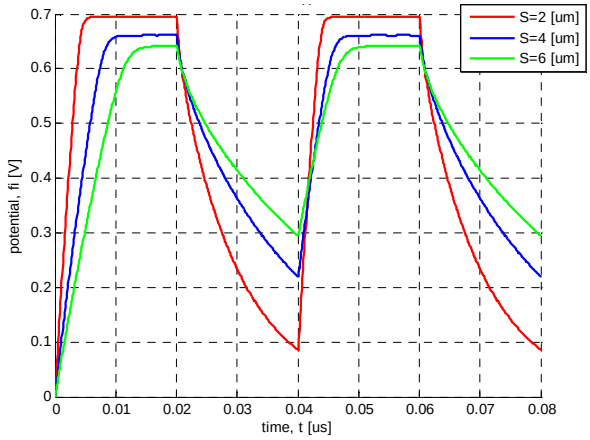
$$i_{fa} = i_{0a} \cdot \sinh(\frac{nF\varphi_a}{2R\theta}) \quad (14)$$

$$q = \int_0^T i_{fa} dt \quad (15)$$

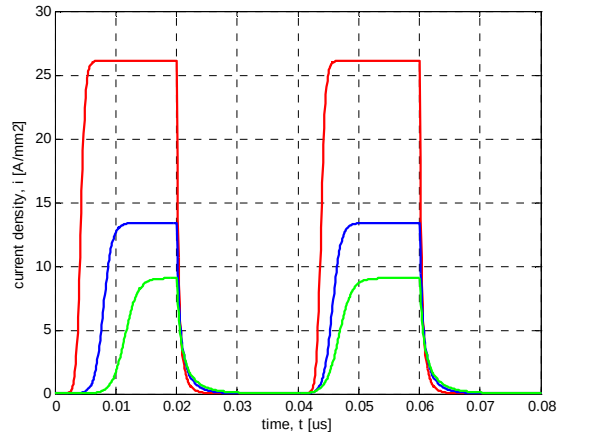
$$\bar{i}_a = \frac{q}{t_p} \quad (16)$$

On basis of the mathematical model, the computer software was developed for simulation of electrode process on anode and cathode in order to calculate $\varphi_a(t)$, $\varphi_k(t)$, $i_{fa}(t)$, $q(t)$ and $i_a(t,S)$. MATLAB's computational procedure and graphic package were applying in this software.

The examples of curves $\varphi_a(t)$, $i_{fa}(t)$, $q(t)$ and $i_a = i_{fa}(t,S)$ determined from computer simulation are shown in Fig. 3.



a)



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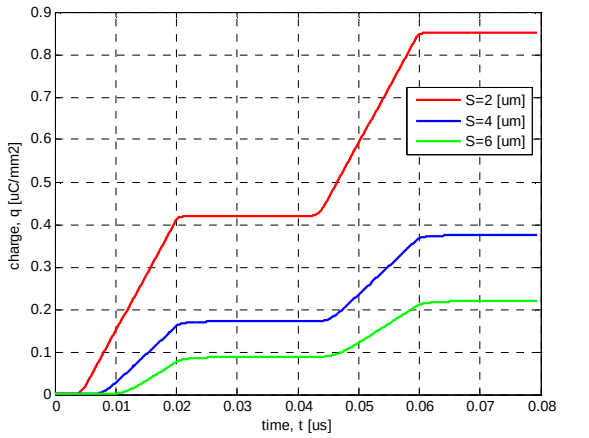

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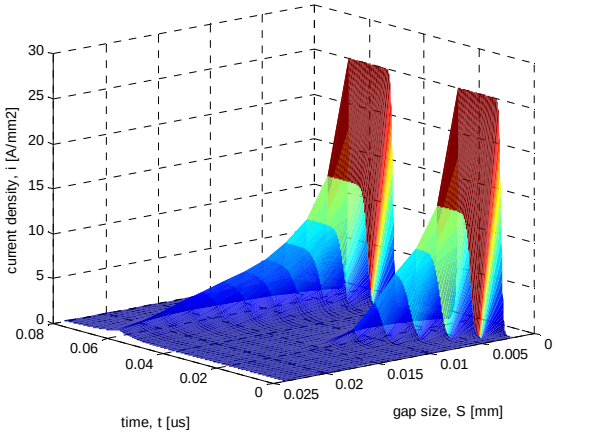


d)

Fig. 3. Example of results of computer simulation of two pulses sequence: changes of anodic potential (a), current density (b, d) and charge (c) in time at gap size S: 0.002 mm, 0.004 mm, 0.006 mm (U = 4 V, t_p = 80 ns, f = 5 MHz, κ = 0.002 V/A·mm, C = 0.2 μF/mm^2, i_0 = 2.5·10^{-5} A/mm^2).

Curves $i_a(t)$ for different gap size are shown in Fig. 4.

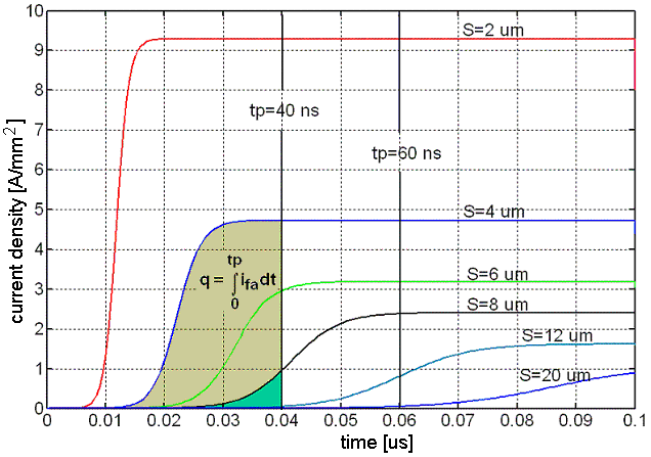


Fig. 4: Anodic current density and electrical charge (U = 5 V, κ = 0.005 V/A·mm, C = 0.2 μF/mm^2, $i_0 = 2.5 \cdot 10^{-5}$A/mm^2).

As shown in Fig. 4, at the certain gap size, the current density is decreasing to no significant value and dissolution is practically stopped. Electrical charge q is equal to area below curve $i_a(t)$. For specified pulse on-time t_p, for example t_p = 40 ns is marked in Fig. 4, surface area is different for particular gap size. Surface area decreases if gap size increases. After exceeding certain gap size, for example t_p = 40 ns for the simulation shown in Fig. 4, the dissolution of workpiece does not proceed for gap size bigger than 12 μm because pulse on-time is too short in order to charge electrical double layer fully. This gap size is called **the limiting gap S_l** because dissolution process stops for the gaps bigger than the limiting gap. With increase pulse on-time t_p to 60 ns (Fig. 4), the limiting gap size increases to 20 μm. As mentioned earlier, the dissolution limiting effect of is important for the localization of material removing, which is necessary for micromachining.

In next part of analysis, the limiting gap S_l were evaluated for different pulse on-time. The limiting gaps S_l for voltage 4 V and 6 V are shown in Fig. 5.

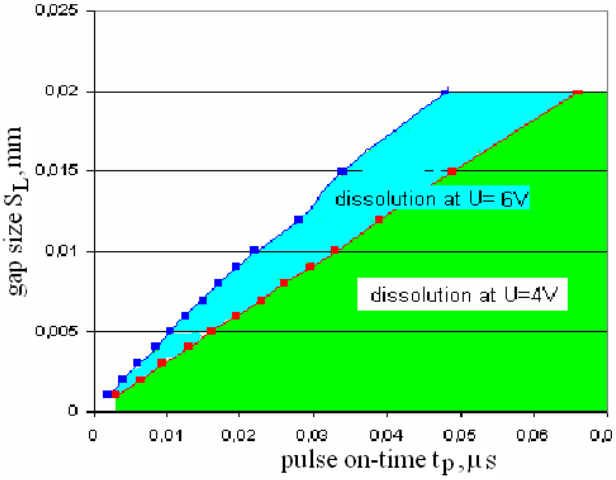
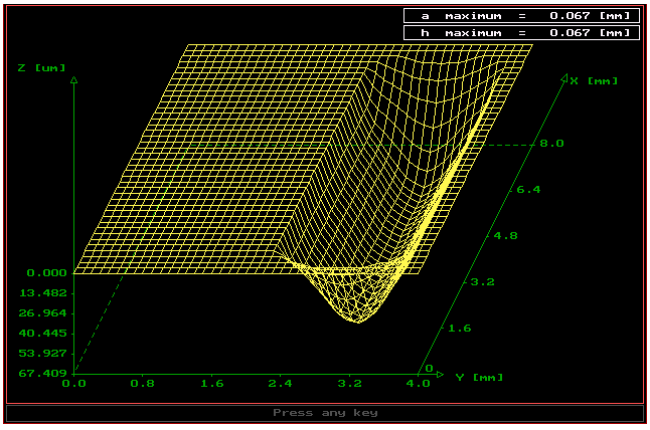


Fig. 5: The limiting gap S_l vs. pulse on-time t_p (C = 0.2 μF/mm^2, κ = 0.005 V/A·mm, $i_0 = 2.5 \cdot 10^{-5}$ A/mm^2)

For example for pulse on-time t_p = 20 ns and voltage U = 4 V, anodic dissolution stops for the gap size bigger than 6 μm. For voltage 6 V and the same pulse on-time, the limiting gap is 9 μm. Influence voltage on the localization of dissolution is shown in Fig. 5. When voltage U increases, the localization is lower (the limiting gap S_l is bigger for the same pulse on-time t_p).

The calculated characteristics of PECMM electrode processes have been used in developed software for simulation of microshaping. Results of simulation can be viewed in two ways: tables of coordinates of points of the workpiece surface for a chosen cross - section perpendicular to x or y axis and 3-D or 2-D graphs.

Figure 5 shows examples of a 3-D graph of the workpiece surface after PECMM machining with two different paths of tool electrode: streamline, curvilinear.



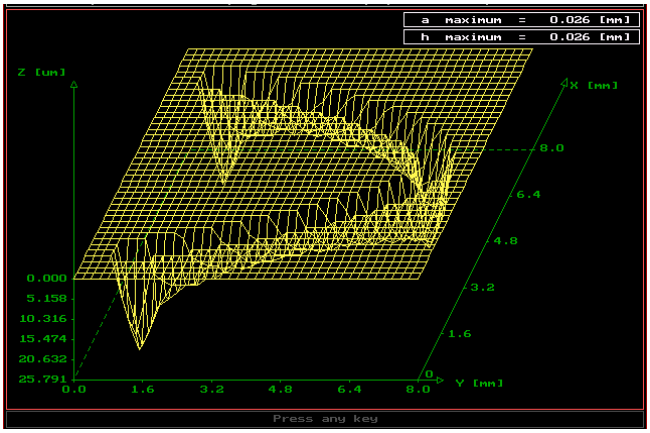


Fig.6: Examples of simulation of electrochemical shaping using streamline and curvilinear path of tool electrode

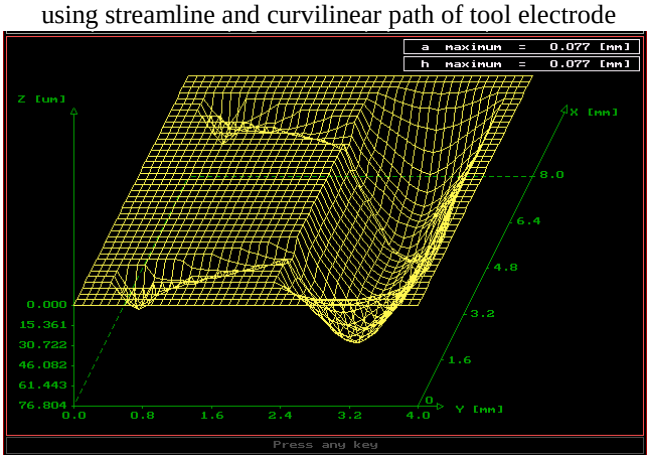


Fig. 7: Shape of machined surface by sequence two path of tool electrode

The final shape of machined surface by using sequence of

the above paths is shown in Fig. 7.

The developed software has been used to determine the influence of machining parameters on final machined shape.

III. Experiments and Results

The PECMM experiment setup is shown in the Fig. 8, respectively. The tool electrode of a diameter of 100 μm has been used for machining the slots of 1.5 mm length, cavities and micro holes on stainless steel (SS-440). The electrolyte used is 10% solution of $NaNO_3$. These microstructures have been generated with the application of 4-8 V pulses of 1-5 MHz frequency, initial interelectrode gap of 20 μm, and tool electrode feed rate of 0.008 -0.013 mm/s.

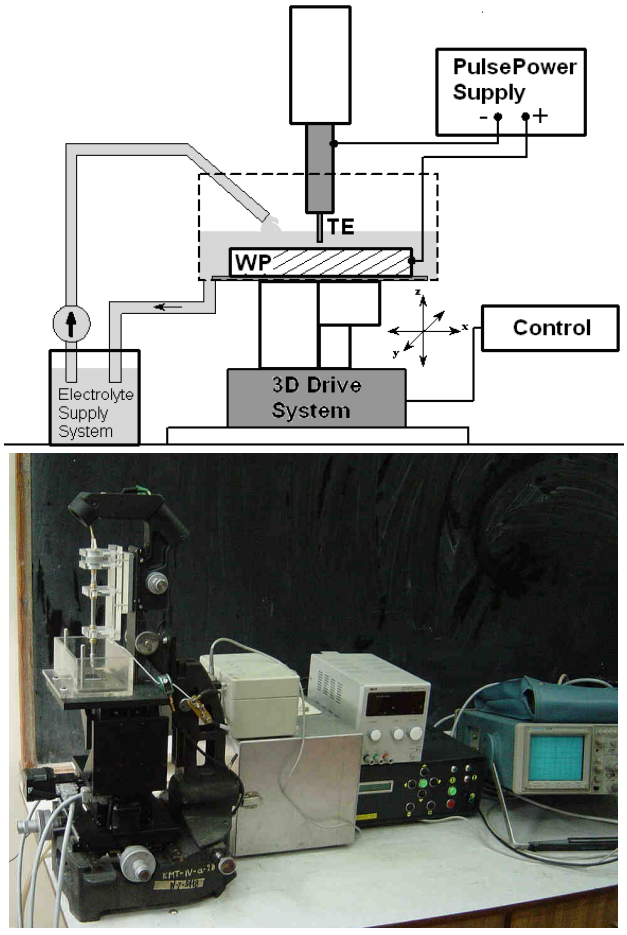


Fig. 8: Schematic diagram and photo of developed Pulse Electrochemical Micromachining system.

The extensive experimental study and subsequent statistical analysis indicate that the feed rate, pulse voltage and pulse on time have significant effect on each of the performance measures. Remaining parameters do not show significant effect on the performance measures. To analyze the effect of these three factors and to verify the theoretical model further experiments were conducted.

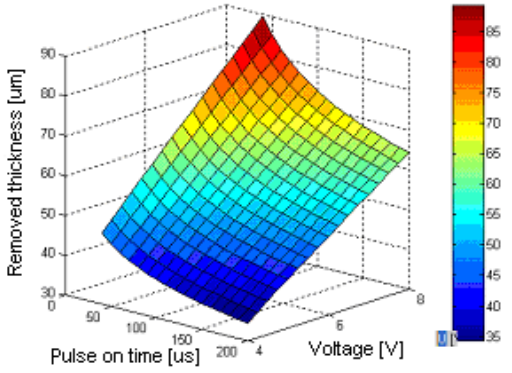


Fig. 9: Removed thickness (depth of hole) vs. pulse on time and voltage.

For example, the results of the effect of voltage, on removed thickness (depth of hole) after machining time of 30 s are shown in Fig. 9. The plot shows that with the increase in voltage the removed thickness increases. The microscopic examination shows that the edges of the machined cavity are sharper at the lower voltage values.

The strategy used for the verification is the comparison of the relative changes in the removed thickness W_t obtained experimentally with the relative changes in electrical charge q determined from computer simulation. This method is adopted because the coefficient of electrochemical machinability K_V is unknown for nanosecond pulses. Then the graph is plotted for non dimensional values the W_t/W_b and q/q_b, where W_b and q_b are the reference base level. The reference values W_b and q_b have been determined for the same base setting parameters of experiments and calculations (U_b = 6 V, S_b = 15 μm, t_b = 100 ns).

The results of comparisons are shown in Fig. 10.

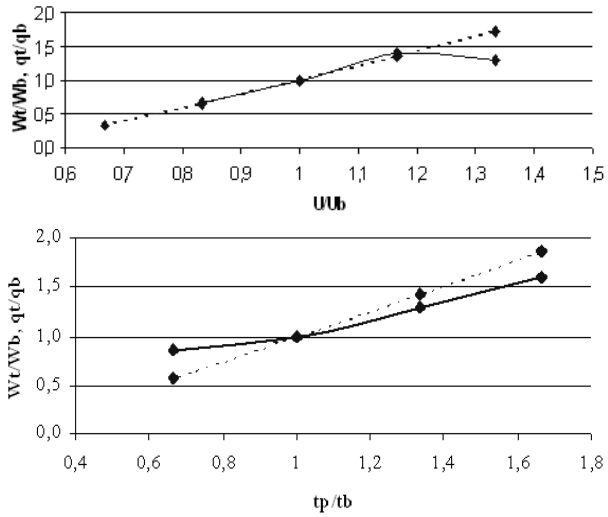


Fig. 10: The comparisons of theoretical (solid line) and experimental results (dashed line).

A close agreement between the theoretical estimates and experimental values has been observed.

IV. Conclusions

Transient phenomena connected with charging and discharging electrical double layers, which exists on boundaries: workpiece – electrolyte and tool electrode –

electrolyte have important role in electrochemical micromachining with ultrashort pulses.

The developed mathematical models and software for simulation of electrochemical micromachining with ultrashort voltage are useful for analysis of electrode potential, dissolution current and electrical charge during PECMM machining with set conditions and allows determination of the influence process conditions on the localization of anodic dissolution and performance characteristic of PECMM. The developed software for simulation of microshaping is useful for PECMM process analysis, surface shape prediction and optimization.

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