Virtual estimation of the intensity of deformation when producing samples from a magnesium alloy of the composition Mg-1% Ca by SPD methods according to ECAP and HPT schemes

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Abstract: *The application of mathematical methods is one of the most rational approaches used to solve tasks of evaluating the efficiency of unconventional metal forming processes. Using computer simulation in the DEFORM-3D application software package, we performed virtual full factorial experiments for the processes of producing individual samples by equal-channel angular pressing (ECAP) and high-pressure torsion (HPT) from the Mg-1%Ca magnesium alloy, taking assumptions into account. At the stage of the simulation task preparation, it was accepted that the most significant factors that influence the fabrication of defect-free semi-products by severe plastic deformation (SPD) via ECAP are the processing temperature and the number of processing cycles via route Bc. In both models, strain intensity was taken as the response parameter. To simulate the SPD process of HPT, the processing temperature and the number of revolutions were used as the main variable factors. In the virtual full factorial experiment, the effect of independent factors on strain intensity was evaluated. As a result of the experiments, regression equations were obtained, variants of the rational processing regimes for the investigated alloy were presented, and their effect on the response parameter was analyzed. The proposed and implemented numerical models allow us to recommend the ECAP processing of the Mg-1%Ca magnesium alloy at a deformation speed of 1.0 mm/s and temperature of about 350 °C for 2 – 4 cycles, and the HPT processing under a hydrostatic pressure of 6 GPa at room temperature with the number of revolutions from 3 to 5.*

KEYWORDS: *COMPUTER SIMULATION, Mg-1%Ca MAGNESIUM ALLOY, VIRTUAL FULL FACTORIAL EXPERIMENT, STRAIN INTENSITY.*

1. Introduction

In recent years, a special interest has been aroused by producing ultrafine-grained (UFG) and nanocrystalline (NC) states in metallic materials by means of deformation treatment aimed at strength enhancement. An important task is to provide the conditions for the deformation-induced increase in strength due to the formation of UFG and/or NC states together with a homogeneous distribution of nano-sized particles [1, 2].

For instance, authors in [3-5, etc.] report the results from the studies of the mechanical properties of magnesium alloys depending on the microstructure produced by severe plastic deformation (SPD), in particular, by equal-channel angular pressing (ECAP) and high-pressure torsion (HPT). A high efficiency of the deformation methods has been demonstrated for increasing the strength of the investigated Mg alloys.

It has been noted that the most common SPD techniques used for producing bulk UFG and NC billets and samples are ECAP and HPT.

These techniques enable producing UFG and NC objects [6], providing an accumulated strain of $e \approx 1$ in one processing cycle.

Against the background of research in the strain hardening of metals, study of the effect of grain size on the functional properties of metallic materials with a bulk UFG and NC structure is of great scientific and practical interest.

SPD techniques, in particular, ECAP [1] and others, enable increasing the strength of alloys by 20 – 60% and the strength of pure metals by a factor of 1.5 – 2, through the formation of a UFG and NC structure.

Technical processes based on structure refinement by SPD processing are especially relevant for increasing the strength of Mg-based materials aimed at their use in biodegradable medical implants for osteosynthesis. Mg alloys are attractive due to their high damping properties, low specific weight, high biocompatibility and hypoallerginicity. However, at the research stage, using the above-mentioned techniques, it is necessary to solve the task of selecting the rational processing regimes for producing individual samples.

In the scientific and practical activities, in important place is held by the numerical methods for the study of complex processes, including computer simulation with the use of the cutting-edge software [7-9]. The efficiency of using simulation methods and solving engineering tasks considerably increases if conditions for the evaluation of the most important independent factors are created at the stage preceding the design of an actual technological process.

The application of mathematical methods is one of the most rational approaches used to solve tasks of evaluating the efficiency of unconventional metal forming processes. In this connection, it appears rational to perform numerical simulation with the use of a virtual full factorial experiment (FFE) [10].

The advantage of an FFE is the capability to describe a process fully observing the algorithm of a physical experiment with the consideration of the assumptions. Among the methods of physical experiment, the FFE is the most easily implementable one. The aim of using an FFE is to obtain a linear mathematical model of a process that will enable deciding on the subsequent strategy of an actual experiment.

Therefore, the aim of the simulation is to perform the virtual process of SPD via ECAP and HPT with the use of an FFE, and to determine the rational number of processing cycles and the temperature regimes for the fabrication of individual samples.

2. Experimental

To obtain the fullest possible information about the relationships under investigation, the authors used an FEE during the simulation. Design of experiments is a procedure of selecting the number and conditions of experiments necessary and sufficient to obtain the mathematical model of a process [11]. The following should be taken into account: the striving for the minimization of the number of experiments; a simultaneous variation of all the variables defining the process; the choice of a clear strategy that enables making grounded decisions after each series of experiments. Prior to the design of a full-scale experiment, it is necessary to collect additional information about the object of study using the skills and knowledge obtained earlier in previous research or described in literature [12].

The design of the experiments was carried out on the basis of the simulation of the process of producing individual samples from the Mg-1% Ca magnesium alloy by ECAP and HPT. The principles of these processes are presented in Figs. 1 and 2.

The object of study was the Mg-1%Ca magnesium alloy. When developing the numerical model, its rheological properties were taken based on the data presented in [13, 14].

To implement the numerical simulation procedure, the standard applied software package *DEFORM-3D* was employed.

In order to perform the simulation and the factorial experiment in *DEFORM-3D*, 3-D models had previously been created using the *Kompas-3D* software.

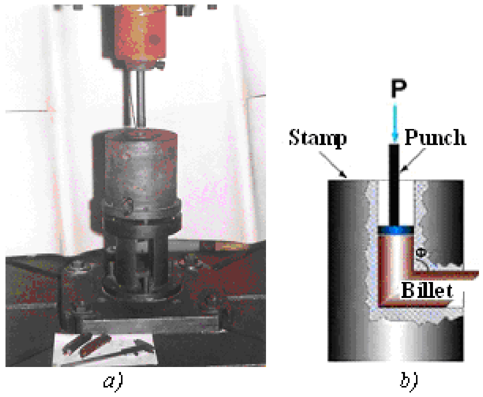

Fig. 1. ECAP facility and die-set: a) – facility for SPD processing by ECAP; b) – test principle

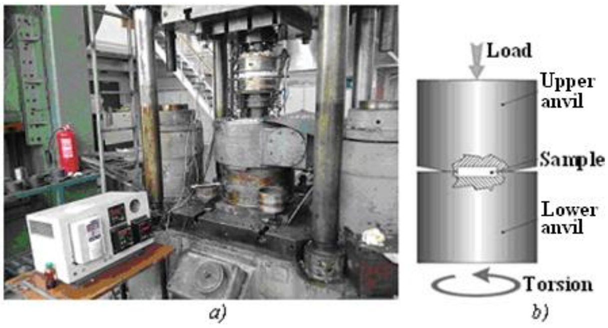

Fig. 2.: HPT facility and die-set: a) – facility for SPD processing by HPT; b) – test principle

2.1.1. Assumptions for the ECAP process model:

1) The billet material in the initial state is isotropic and lacks initial stresses and strains;
2) The processing temperatures are taken as *250 °C* and *450 °C*;
3) The channels intersection angle is *120°*;
4) The tool is absolutely rigid, and the tool geometry is taken into account automatically;
5) The initial billet material is taken as ductile;
6) *100* steps are chosen for the simulation, taking into account the complete passage of the billet and the generation of a stable result;
7) The billet is divided into *43553* trapezoidal elements;
8) The friction factor (according to Siebel) in the deformation site is *0.3*;
9) The billet diameter is 20 mm;
10) The billet length is 100 mm;
11) The processing speed is 1.0 mm/s.

2.1.2. Assumptions for the HPT process model:

1) The billet material in the initial state is isotropic and lacks initial stresses and strains;
2) The processing temperatures are taken as *20 °C* and 1*50 °C*;
3) The tool is absolutely rigid, and the tool geometry is taken into account automatically;
4) The initial billet material is taken as ductile;
5) The billet divided into 55000 trapezoidal elements;
6) The friction factor (according to Siebel) in the deformation site is 0.95;
7) The rotation speed of the upper anvil is 1 rev/min;
8) The pressure is *P = 6 GPa – Const.;*
9) The sample diameter is 20 mm;
10) The sample thickness is 1.4 mm.

2.2. Procedure of preparation for the simulation

At the stage of the preparation of the simulation task we consider that the most significant factors influencing the fabrication of defect-free semi-products by SPD processing via ECAP are the processing temperature and the number of processing cycles via route Bc (where the billet is rotated 90° with respect to its longitudinal axis after each processing cycle). The response parameter is strain intensity.

To simulate the SPD process of HPT, we shall accept the processing temperature and the number of revolutions as the main variable factors. The response parameter is strain intensity. This parameter can be evaluated with the help of a model and then verified in an actual experiment through a direct measurement of the force parameters and the testing of the mechanical properties (microhardness) with the analysis of the structural state.

In this connection, it was decided to perform the virtual FFEs using two-level models with two unknowns in consistency with the number of the variable factors. Formalization of the obtained results in the form of regression equations and the subsequent optimization of the chosen variable factors will enable selecting the rational regimes of processing by both techniques, taking into account the assumptions.

Thus, the processing temperature ***(X_1)*** and the number of processing cycles ***(X_2)*** were selected as the independent variables in the SPD process of ECAP, characterizing the efficiency of the process in terms of strain intensity. Strain intensity ***(Y_{ECAP})*** was taken as the response parameter (the dependent parameter).

To simulate the HPT process, the number of revolutions ***(X_1)*** and the processing temperature ***(X_2)*** were taken as the variable factors. The response parameter was also strain intensity ***(Y_{HPT}).***

The factors were varied in two levels. The variation ranges of the variable factors for the ECAP process and their values in full scale are shown in Table 1.

Table 1 Factor levels in the simulation of ECAP

Factors	X_1 *(T, °C)*	X_2
Basic level (X_i)	350	1
Variation range (ΔX_i)	100	1
Upper level (x_i = + 1)	450	4
Lower level (x_i = – 1)	250	1

The ranges of the two-level variation of the variable factors for the HPT process and their values are shown in Table 2.

Table 2 Factor levels in the simulation of HPT

Factors	X_1, rev.	X_2, *(T, °C)*
Basic level (X_i)	3	100
Variation range (ΔX_i)	0.5	10
Upper level (x_i = + 1)	5	150
Lower level (x_i = – 1)	0.5	20

The number of experiments, *N*, was found from the number of factors, *k*, in accordance with the relation:

$$N = 2^k = 2^2 = 4. \tag{1}$$

It is necessary to find such values of X_1 and X_2 that provide the highest strain intensity.

3. Experiment results and discussion

3.1. Simulation of the SPD process of ECAP

After implementing the full factorial experiments, the mathematical model will have the following view:

$$y=b_0+b_1x_1+b_2x_2+\ldots+b_{12}x_1x_2, \tag{2}$$

where b_i is the regression coefficient.

To calculate the coefficients of this model, we used an extended matrix of experiment design and results (Table 3).

Table 3. *Extended matrix for the design 2^2 and results of the virtual experiments*

	X_o	X_1	X_2	X_1X_2	Y_{ECAP} (average values)
1	+	+	+	+	2.87

2	+	-	+	-	3.00
3	+	+	-	-	0.59
4	+	-	-	+	0.71

Taking into account the accepted conditions and assumptions, Fig. 3 shows the solution for the tasks of the numerical simulation of the ECAP deformation process, as a result of which the strain intensity values were obtained.

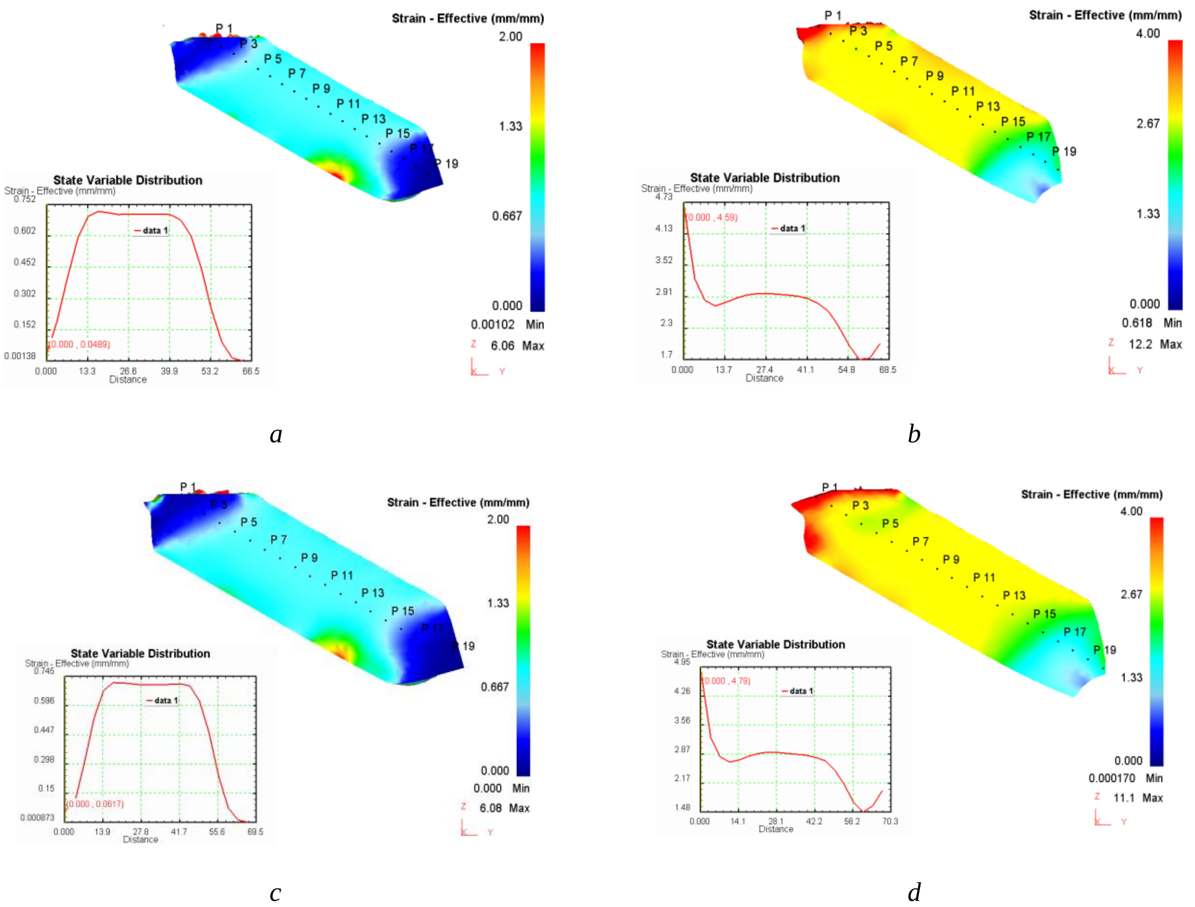

Fig. 3. *Results of finding the strain intensity values, obtained during the simulation of the ECAP deformation process: a – 1 processing cycle at a temperature of 250 °C; b – 1 processing cycle at a temperature of 450 °C; c – 4 processing cycles at a temperature of 250 °C; d – 4 processing cycles at a temperature of 450 °C*

The regression equation demonstrates the effect of the accepted variable factors on the response parameter – strain intensity:

$$Y_{ECAP} = 1.79X_o - 0.063X_1 + 1.143X_2 - 0.0025X_1X_2. \qquad (3)$$

It can be seen from the obtained regression equation that the number of deformation processing cycles has the largest effect on strain intensity. The processing temperature has a much smaller effect. There is tendency for a decrease in the processing temperature aimed at some increase in strain intensity. A simultaneous change in the temperature and the number of ECAP processing cycles also has a weak effect. Thus, in the accepted simulation conditions strain intensity primarily depends on the number of deformation processing cycles.

As a conclusion, the simulation of the SPD processing of the Mg-1%Ca magnesium alloy by ECAP allows us to note that processing temperature has a weak effect on strain intensity. At the same time, the number of processing cycles promotes a considerable increase in strain intensity.

3.2. Simulation of the SPD process of HPT

To calculate the coefficients of the model of the virtual full factorial experiment in accordance with formula (2), we used an extended matrix of experiment design and results (Table 4).

Table 4. *Extended matrix for the design 2^2 and results of the virtual experiments*

	X_o	X_1	X_2	X_1X_2	Y_{HPT} (average values)
1	+	+	+	+	7.82
2	+	-	+	-	2.97
3	+	+	-	-	6.14
4	+	-	-	+	4.91

Taking into account the accepted conditions and assumptions, Fig. 4 shows the solution for the task of numerical simulation of the HPT deformation process, as a result of which the strain intensity values were obtained.

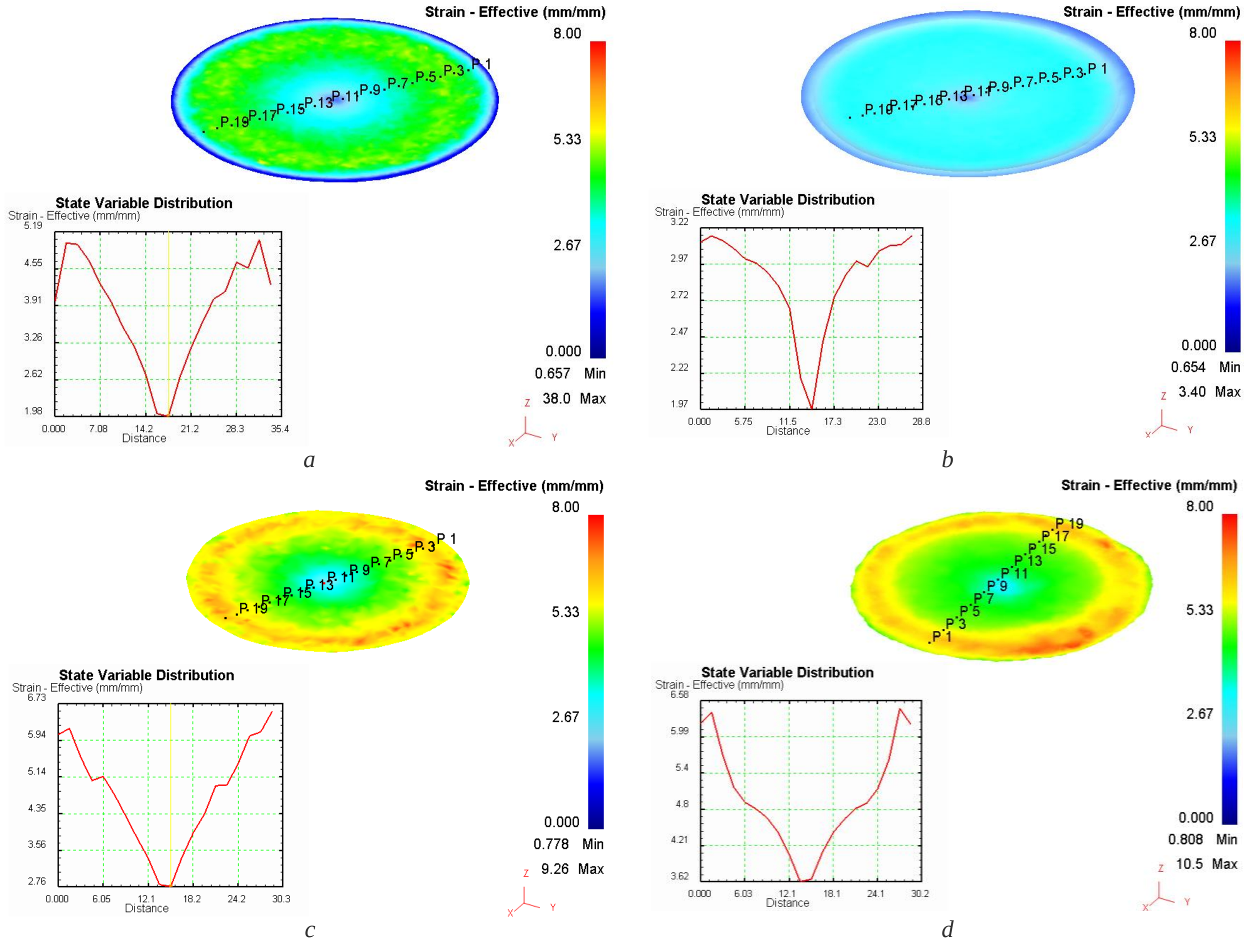

Fig. 4. *Results of finding the strain intensity values, obtained during the simulation of the HPT deformation process: a – 0.5 revolutions at a temperature of 20 °C; b – 0.5 revolutions at a temperature of 150 °C; c – 5 revolutions at a temperature of 20 °C; d – 5 revolutions at a temperature of 150 °C*

The regression equation given below, obtained by numerical simulation, demonstrates the effect of the number of revolutions and temperature on strain intensity during HPT processing.

$$Y_{HPT} = 5.56\,X_o + 1.52\,X_1 - 0.065\,X_2 + 0.91\,X_1X_2. \qquad (4)$$

It follows from the analysis of the obtained regression equation that the number of revolutions of the upper anvil under a constant hydrostatic pressure and a decreased temperature have the largest effect on strain intensity. A simultaneous change in both of the variable factors (an increase in the number of revolutions and a decrease in temperature) also leads to an increase in strain intensity. However, in the case of a small number of revolutions (0.5 revolutions) at temperatures of 20 °C and 150 °C strain intensity is somewhat higher at the lower temperature. As the number of revolutions increases to 5, strain intensity grows significantly even at a temperature of 150 °C, and is much higher than that at 20 °C.

This confirms the adequacy of the proposed model and allows us to recommend the HPT processing of the Mg-1%Ca magnesium alloy at room temperature with the number of revolutions from 3 to 5. A practical experiment will allow us to refine the presented model in the future.

CONCLUSIONS

1. As a result of the virtual full factorial experiment for the simulation of the ECAP processing of the Mg-1%Ca magnesium alloy, we note that processing temperature has a weak effect on strain intensity. The number of processing cycles promotes a considerable increase in strain intensity.
2. The recommended regime of the SPD processing of the Mg-1%Ca magnesium alloy by ECAP at a deformation speed of 1.0 mm/s is a temperature of about 350 °C for 2 – 4 cycles.
3. In the SPD processing by HPT, the number of revolutions of the upper anvil under a constant hydrostatic pressure and a decreased temperature have the largest effect on strain intensity. A simultaneous change in both of the variable factors (an increase in the number of revolutions and a decrease in temperature) also leads to an increase in the strain intensity values.
4. The preliminary simulation results demonstrate the adequacy of the developed model which needs to be refined by a full-scale experiment for the SPD processing of the Mg-1%Ca magnesium alloy by ECAP and HPT.
5. The proposed and implemented model allows us to recommend the HPT processing of the Mg-1%Ca magnesium alloy under a hydrostatic pressure of 6 GPa at room temperature with the number of revolutions from 3 to 5.

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References

1. R.Z. Valiev, A.P. Zhilyaev, T.G. Langdon, Bulk Nanostructured Materials: Fundamentals and Applications, 2014 by John Wiley & Sons, Inc., 456 pages.

2. R.Z. Valiev, I.V. Alexandrov, Nanostructured Materials Produced by Severe Plastic Deformation, 2006, Science Press, 151 p. (in Chinese).

3. S.V. Dobatkin, L.L. Rokhlin, T.V. Dobatkina, Lukyanova. Structure and mechanical properties of a Mg-Y-Gd-Zr after severe plastic deformation//Technology of Light Alloys. – 2015. – № 2. – P. 23-29 (in Russian).

4. S.V. Dobatkin, L.L. Rokhlin, G.A. Salishchev, V.I. Kopylov, V.N. Serebryany, N.D. Stepanov, I.E. Tarytina, I.S. Kuroshev, N.S. Martynenko. Structure and properties of an Mg-0.3%Ca magnesium alloy after multiaxial deformation and equal-channel angular pressing//Russian Metallurgy (Metally). –2014.–№ 214.– P. 911-919.

5. A.Yu. Vinogradov, E.V. Vasil'ev, M.L. Linderov, D.L. Merson, E.O. Rzhevskaya. Effect of equal-channel angular pressing on the structure and mechanical properties of Mg-Zn-Ca magnesium alloys//Science Vector of Togliatti State University. – 2015. – № 4 (34). – P. 18-24 (in Russian).

6. V.M. Segal, V.I. Reznikov, V.I. Kopylov, et al. Processes of Plastic Structure Formation in Metals. Minsk: Nauka i Tekhnika, 1994. 232 p. (in Russian).

7. V.I. Semenov, S.-J. Huang, L.Sh. Shuster, A.G. Raab Computer Simulation of Continuous SPD Process Commercially Pure Titanium Using Virtual Full Factorial Experiment with the Influence of Friction Factors// ISSN: 0354-8996 Tribology in Industry, Vol. 38, No. 1 (2016) 127-132.

8. V.V. Kamburov, V.I. Semenov, N.T. Tontchev, V.P. Mishev, A.A. Nikolov 3D Simulation by CAD/CAE software of deformation process at equal-channel angular extrusion with active friction forces//Proceedings of 14th In. Sc. Cong. «Machines, Technologies, Materials», Varna, Bulgaria, Sept. 13-16, 2017, V. VI (6), 2017, ISSN print 2535-0021, ISSN web 2535-003X, pp. 423-426.

9. A. Belhocine, A.R. Abu bakar, M. Bouchetara Numerical Modeling of Disc Brake System in Frictional Contact//Tribology in Industry, Vol. 36, No. 1 (2014) 49-66.

10. F.S. Novik, Ya.B. Arsov, Optimization of the Metals Engineering Processes by Design of Experiments. -Moscow: Mashinostroenie; Sofia: Technika. 1980. 304 p. (in Russian).

11. Yu.P. Adler, Design of Experiments. -Moscow: Znanie. 1978. 72 p. (in Russian).

12. Yu.P. Adler, Introduction to the Design of Experiments. Moscow: Metallurgiya. 1969. 158 p. (in Russian).

13. O. Kulyasova, R.K. Islamgaliev, B. Mingler, M. Zehetbauer. Microstructure and fatigue properties of the ultrafine-grained AM60 magnesium alloy processed by ECAP. Mat. Sci. Eng. A503 (2009) 176-180.

14. Li, Z., et al. The development of binary Mg–Ca alloys for use as biodegradable materials within bone. Biomaterials, 2008. 29 (10): p. 1329-1344.