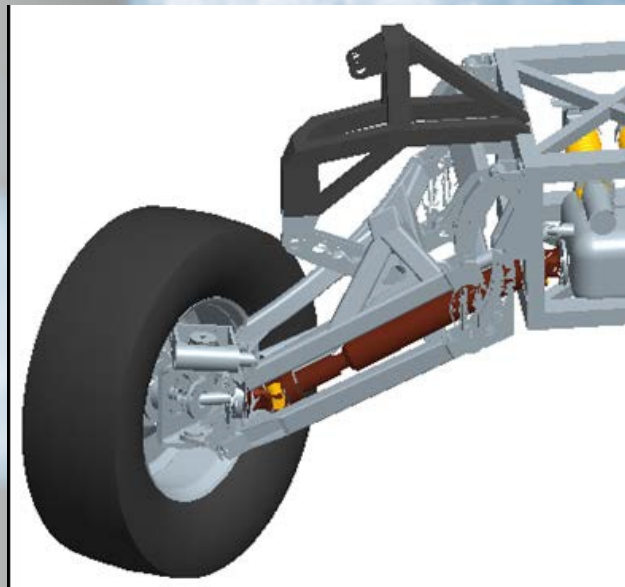


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CONTENTS

MACHINES

DESIGN PROCESS FOR THE SUSPENSION SYSTEM OF THE TERRAIN VEHICLE WITH FOUR WHEEL DRIVE

Asoc. Prof. Dr. Naser Lajqi, Asoc. Prof. Dr. Azem Kyçyku, Ass. Prof. Dr. Shpetim Lajqi 477

MARINE SLOW SPEED TWO-STROKE DIESEL ENGINE - NUMERICAL ANALYSIS OF EFFICIENCIES AND IMPORTANT OPERATING PARAMETERS

PhD. Mrzljak Vedran, Student Žarković Božica, Prof. PhD. Prpić-Oršić Jasna 481

TECHNOLOGIES

MULTILEVEL MODIFICATION IN MATERIALS SCIENCE AND POLYMER NANOCOMPOSITES TECHNOLOGY

Assoc. Prof. cand. eng. Avdeychik S., Senior lecturer Antonov A., Prof. Dr. Eng. Struk V., Assoc. Prof. cand. eng. Vorontsov A., Assoc. Prof. cand. eng. Abdurazakov A. 485

DETERMINING OF STORAGE SITE LOCATION WITHIN PRODUCTION SYSTEMS

Associate Prof. Topčić A. PhD., Associate Prof. Cerjaković E. PhD., Assistant Prof. Lovrić S. PhD., M.Sc. Herić M. 490

pH AND TEMPERATURE INFLUENCE ON PHENOL REMOVAL FROM WATER BY HORSERADISH PEROXIDASE

PhD Savic S., PhD Petrovic S., Phd stud. Petronijevic M., Prof. Dr. Petronijevic Z. 494

FULL USE OF MATHEMATICS – FOUNDRY

Bushev S., Associate Professor, PhD, Eng. 497

THE METHODOLOGY FOR VEHICLES PARKING ANALYSIS: CASE STUDY – CITY OF PRISHTINA

Assoc. Prof. Dr. Lajqi Naser, Ass. Prof. Dr. Lajqi Shpetim, Prof. Dr. Doçi Ilir 499

MODELING OF SOLIDIFICATION IN RESISTANCE SPOT WELDING

Jafari R. PhD. 504

MATERIALS

EFFECT OF ANNEALING TEMPERATURE ON MICROSTRUCTURE OF Ti-Al-V-Mo-Zr SYSTEM ALLOYS

Doctor of Engineering Sciences Terlikbayeva A. Zh., 3rd year PhD student Alimzhanova A.M., Candidate of Engineering Sciences Shayachmetova R.A., Candidate of Engineering Sciences Ossipov P.A., Doctor of Engineering Sciences, professor Smagulov D.U. 505

WEAR RESISTANCE OF CARBIDE-BAINITE SPHEROIDAL GRAPHITE CAST IRONS UNDER CONDITIONS OF DRY FRICTION

Assist. Prof. Vladimir Todorov, Assoc. Prof. Georgi Rashev, eng. Milen Svilenov 509

GRADIENT INTERFERENCE OPTICAL FILTERS MANUFACTURED FROM ORGANOSILICONE COMPOUNDS WITH THE RF PECVD TECHNIQUE

Katarzyna Oleško, MS; Hieronim Szymanowski, PhD, DSc; Prof. Maciej Gazicki-Lipman, PhD, DSc; Anna Sobczyk-Guzenda, PhD. 512

DESIGN PROCESS FOR THE SUSPENSION SYSTEM OF THE TERRAIN VEHICLE WITH FOUR WHEEL DRIVE

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Abstract: This paper discusses the research methodologies utilized for developing a suspension system for a four wheel-drive terrain vehicles. The main research methods can be identified as literature studies; design processes by applying CAD systems, numerical analyses methods, mathematical modeling and simulation, optimization of the mechanical systems, as well as the comparison, analysis, and evaluation of the obtained results. The proposed suspension system for the terrain vehicle was successfully derived at from a classic double wishbone control arm. Optimization of the suspension parameters for passive ones is performed by Multi Objective Genetic Algorithms, whilst for active damping force by employing Hooke-Jeeves non-linear programming method. On the basis of comprehensive analysis it is shown the active systems are more adequate. The proposed suspension design provides relatively small lateral wheel motion, zero camber angles, and effectively absorbs the vibrations caused by road excitation.

Keywords: DESIGN, SUSPENSION SYSTEM, OPTIMIZATION, MODELING, CAD

1. Introduction

The primary function of the vehicle's suspension system is to keep quality contact between the tires and the road surface, as well as to isolate the vehicle's body from vibration coming from road disturbances. The suspension system physically connects the vehicle's chassis with its wheels, and consists of wheels with tires, springs, shock absorbers, and a few rods and linkages, as well as the steering system, Lajqi [1], Lajqi et al. [2, 3].

Scientific papers, patents, many original and innovative concepts regarding suspension have been studied and analyzed by different authors.

Mokhlespour et al. [4] in their research, present an optimization procedure for a double wishbone suspension system with variable camber angle adjusting of hydraulic mechanism.

Allred [5] explores how a compliant mechanism can be used within vehicles' suspension system. Such a mechanism has advantages regarding the questions of space requirements, lower number of joints, rigid links, and simpler design for manufacturing and assembly.

Heo et al. [6] have developed a method for computing kingpin geometry which is an important design feature of vehicle suspension geometry. The idea of a geometric kingpin axis has been used to design a relatively simple suspension mechanism such as a double wishbone type, and various techniques have been developed for designing the kingpin axes of multi-link suspensions.

Maher [7] has identified control strategies for vehicle suspension system by measuring operational data. Finding methods for identifying the values of suspension parameters has considerable interest, in practice. For facilitating experimental suspension system data, a quarter car suspension test rig has to be constructed.

Bouzara and Richard [8] have analyzed the effects of vibrations on the driving comfort and driving safety observed by a variation of different suspension coefficients, road disturbances, and seating positions. In their study they developed a mathematical model for simulating the dynamic behavior of a 3-D vehicle.

Gobbi and Mastinu [9] have used a simple linear model to derive at a number of analytical formulas that describe the dynamic behavior of the passive suspension system. They have introduced an optimization method, based on Multi-Objective Programming and Monotonicity analysis featuring the best compromises between those conflicting objective functions that indicate improved driving comfort, driving safety, and suspension travel.

Baumal et al. [10] demonstrated numerical optimization methods for partially automating the design process. A global

optimization technique such as Genetic Algorithms is used to determine vehicle suspension parameters. Genetic Algorithms are also used to compare obtained results from cited literature based on a gradient projection method.

Alkhatib et al. [11] has used the Genetic Algorithms method for optimizing the problem of a linear vibration isolator. This method was extended to optimize a linear quarter vehicle model.

Yu and Yu [12] describe a procedure for obtaining an optimal vehicle suspension design on a quarter vehicle dynamic model. Two objective functions were used for minimizing the acceleration of the sprung mass and suspension travel, subject to a number of constraints. In solving this problem, the Genetic Algorithms have been used and consistently found to be near optimal solutions within specified parameter ranges for several independent runs.

The proposed suspension system for the terrain vehicle was successfully derived at from a classic double wishbone control arm. The control arms are long but both equal. Larger wheel motion is ensured without reducing driving performance. To improve the comfort and safety an optimal active damping force is determined by the active and semi-active systems. Optimization of the suspension parameters for passive ones is performed by Multi Objective Genetic Algorithms, whilst for active damping force by employing Hooke-Jeeves non-linear programming method. On the basis of comprehensive analysis it is shown the active systems are more adequate. The proposed suspension design provides relatively small lateral wheel motion, zero camber angles, and effectively absorbs the vibrations caused by road excitation.

2. Design processes by applying CAD systems

Design processing forms a major part of research and development activities. This process covers the activities of preparing drawings, detailed technical specifications, as well as necessary information for manufacturing products in order to satisfy customer requirements.

Generally speaking, the task of each engineer is to apply his/her scientific and engineering knowledge to find one or more suitable solutions for specific design problems. In addition to the basic design, it is necessary to optimize it according to requirements and constraints; such are materials, technological possibilities, reasonably cost, legal restrictions, and environmental and human source-related considerations.

The design task becomes clearer after recognition of the problem and defining the criteria and requirements that engineers have to adopt and apply in order to design for production.

According to Pahl et al. [13], Mastinu et al. [14] the four stages of the design process can be defined as is shown in Figure 1.

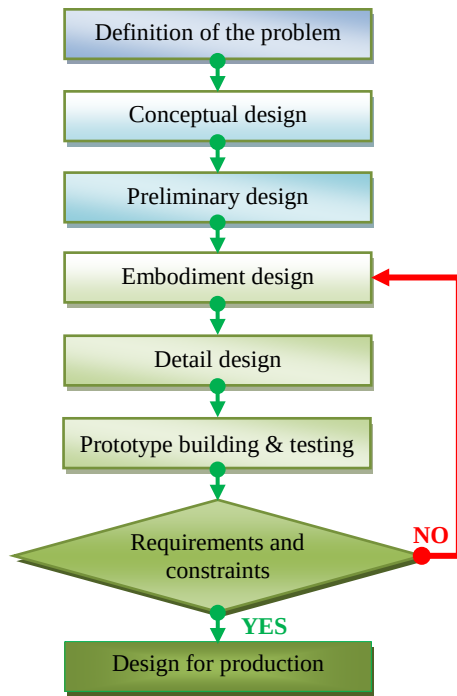


Figure 1. Flowchart diagram showing the stages of the design process

Conceptual design is the part of the design process that determines the method of solving and treating a problem. At this stage it is necessary to identify the essential problems, establish the functions, and find working principles for the problem. The basic solution could be reached by examining the working principles of the problem and combining them with real possibilities, in order to find a solution.

Preliminary design is the second stage of the design process, also known as feasibility design, and is considered as part of the conceptual design. The preliminary design is obtained by refining the conceptual design according to the design specifications regarding the best choice for the preliminary design.

Embodiment design starts from preliminary layouts, selecting the most desirable preliminary layouts, the working concepts of a technical product, and again refining and evaluating using technical and economic criteria. Much work is then done to refine the concept. The geometry, shapes, weights, and interactions are determined during this stage.

Detail design is the final stage of the design process that combines the embodiment of technical products with final instructions for manufacturing. This stage of design includes detailed explanations about the drawings, dimensions, tolerances, sizes, forms, surface properties of all the individual components, specifications of the materials, operating procedures, manufacturing costs, etc.

The classification of the design process as four stages is not a unique one and is in fact a general classification when considering complex mechanical systems. Nowadays, CAD systems are employed for implementing the design phases mentioned previously. The more up-to-date the greater those applications concerning CAD systems utilize computer software's such as AutoCAD, CATIA, Pro/ENGINEER, SolidWorks, etc.

The working principles of CAD systems are based on interactive computer graphics. The users of CAD systems are

designers who use data for executing commands via various input devices of the computer, and develop images on the output device (monitor screen, printer) for faster and easier designing. The designer with his conceptual design performs a part of the design process, whilst the computer carries out the task most suited to its capability, such as fast calculations, searching, sorting, routine operations, displaying on a monitor, analyses of structural design, printing drawings, Balić [15].

The CAD system has many advantages compared with traditional manual design. It improves the efficiency and quality of work, saves money during design, as well as the manufacturing process. The other advantages of the CAD system could be hard to measure but some of them are: increasing the productivity of design, easy corrections of drawings, repetitive parts of a drawing, virtual reality simulation of the structural design, reducing storage space, etc. In addition to advantages, CAD systems also have some drawbacks, such as a high initial cost, requires adequate training and education of staff for efficient usage, reduction of human resources, etc.

3. Numerical analyses methods

Nowadays, as also in past, numerical analysis through Finite Element Methods (FEM) is significantly used in different engineering fields, such as aerospace, automotive, heavy equipment and machinery, civil engineering, etc. Analysis by mechanical systems often presents difficult engineering tasks because of the high complexities of their geometry on the one hand, and the different applied loads (dynamic load, stiffness, etc.), on the other.

The behavior of these systems can be analyzed by setting the differential equations as a basic principle of the mechanics. The solving of differential equations in many cases is impossible, except in those cases where the geometrical, loading, and boundary conditions of the problem are very simple, and makes possible direct integration, Mecitoglu [16]. On the other hand, the solving of a mechanical problem where the geometry and loading condition are relatively complex is impossible to solve by analytical methods.

This problem successfully can be solved by employing numerical methods. FEM belongs to the class of numerical methods and is one of the more powerful methods for solving a wide-spectrum of engineering problems.

The exact period of early development regarding FEM is very difficult to determine, Sorić [17]. The first publication on FEM appeared from J.H. Argyrisa in 1954. The number of publications referring to FEM is relatively large. Between 1967 and 1999, a total of 467 books were published regarding FEM, Mackerle [18]. According to Sorić [17] and Mackerle [18] the first computer program based on Finite Elements was introduced between 1960 and 1970 and by 2002, 1538 FE codes had been registered.

The design task utilized by Finite Element Analysis (FEA) is to investigate the behavior of a structure which is subjected to specific boundary conditions and loads. In order to make an analysis of the mechanical structures using FEA, the real geometry of the structure first needs to be split into discrete portions, which are known as Finite Elements (FE). Each FE is formed by joining points known as nodes. FE and nodes form a grid so-called a mesh. The quarter suspension system of the terrain vehicles performed by discrete FE is shown in Figure 2.

Usually a FE is a non-linear formed by the joining of two nodes. Each node has the capability to move within six degrees of freedom (when three are displacements and three are rotations), Figure 3.

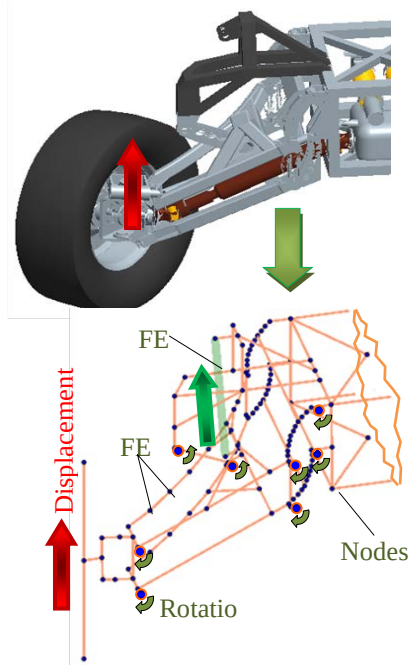


Figure 2. Modeling of a quarter of the suspension system - FE

The relation between the stiffness matrixes, vector displacement, and the applied force in nodes is determined by the global equation of FE. The global equation of FE is described by the following expression:

$$[k] \cdot \{u\} = \{f\}, \quad (1)$$

where $[k]$ denotes the global stiffness matrix of a structure, $\{u\}$ is the global nodal vectors displacement, $\{f\}$ introduces the global nodal vectors of the applied forces, u_i, v_i, w_i are the termed vectors displacement of nodes i_{th} , q_x, q_y, q_z define the rotational vectors of nodes i_{th} in the axes x, y and z and $i = 1, 2, \dots, n$ are the presented nodes.

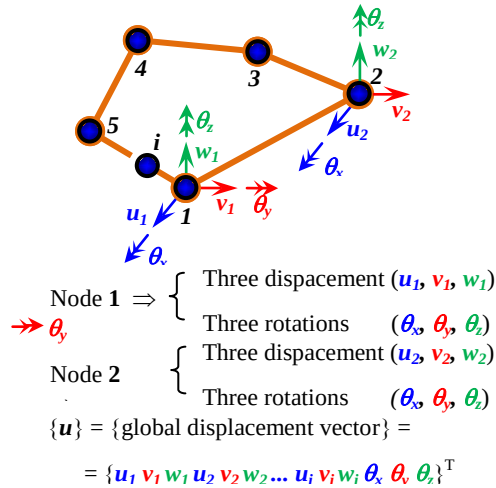


Figure 3. Moving capabilities of FE mapping of nodes

Recently, an improved performance by computers has allowed the rapid development of software packages for solving mechanical problems that are based on FEM.

This software enables modeling, analysis, and optimization, as well as modifications of designs for various engineering problems over a short time. Numerical analysis, dynamic simulation, and optimization can be performed by employing software packages such as STAKx, MATLAB, Working Model, MathCAD, iGOx-i, etc. The tasks of each FEA software is based on FEM formulation

of a model, and the correct defining of input data. In practice, FEA software is usually divided into three parts: pre-processing, processing, and post-processing. A flowchart showing the organization of FEA software, is shown in Figure 4.

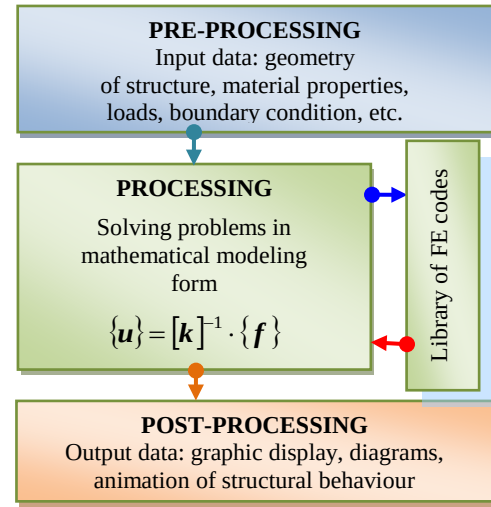


Figure 4. Flowchart diagram of FEA process, [16],[17] and [18]

where $[k]^{-1}$ denotes the global inverse stiffness matrix of a structure. The pre-solver formulates the mathematical model by reading data from pre-processor, the processor computes solution by solving global equation of FE, while in the post-processing stage are presented obtained results and their interpreting.

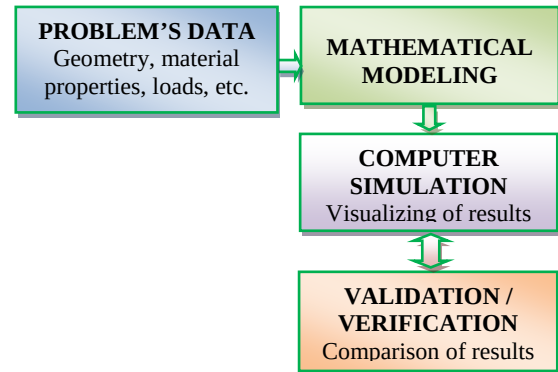


Figure 5. Flowchart of the mathematical modeling and simulation processes

Although mathematical modeling describes just a part of the reality it can be very useful for analyses and design. In most cases when modeling and simulating mechanical systems described using mathematic expressions, software packages such MATLAB/Simulink, MathCAD are used.

4. Optimization of the mechanical systems

Optimization techniques for mechanical systems play an important role. The purpose of this is to find the best ways of deriving maximum benefit from available resources. Over recent years, several optimization methods have been developed (e.g. Gradient, numerical, Genetic Algorithms, etc.). Optimization methods based on Gradient platform are widely used in mechanical optimization systems. These methods have favorable convergence properties and computation effort is very small. However, the optimization method based on Genetic Algorithms is a stronger tool for finding the global optimal point without any requirement on the gradient and the Hessian Matrix. While optimization of the suspension parameters can be done by employing Multi Objective Genetic Algorithms, and the Hooke-Jeeves methods.

Numerical optimization methods that are used in engineering are usually divided into the following three groups, Lenart [19]: conventional, shape and topology optimization methods.

The conventional optimization method is a numerical method and is one of the more popular optimization methods due to its easy usage. This method is based on a modest modification such as the geometric parameters of individual finite elements (e.g. cross-section, thickness, etc.). In other hand, the topology optimization methods are probably the most complex methodology for optimizing mechanical systems and when working intensively to develop. Sometimes shape organization is used between conventional and topological optimization methods. The key problem before shape optimization is the selection of suitable ways for geometric parameterization. The parameterization process used for the optimization of a suspension system is already complex enough. The main reason for this is the fact that the conventional optimization process does not require substantial changes in preparation data for the analysis of the structure. The situation is totally different when optimizing the shape of the suspension mechanism or other structure. Automatically changing FE mesh requires a different concept for preparing geometric data. In this situation, it is necessarily to have several FE codes that have been tested and applied in various applications, and will be used for optimizing the geometry of the suspension mechanism. In this case, the geometric data prepared for modeling the suspension mechanism are so-called project elements obtained from FE codes. These project elements are prepared in ways that depend on the design variables. Design variables, within this context, can therefore be considered as a form of parameterized FE mesh, and the whole approach is called the concept of suspension mechanism parameterization.

5. Optimization method based on a Genetic Algorithms

The Genetic Algorithms (GAs) used for optimization of the mechanical system are stronger tools for finding the global optimal point without any requirement on the gradient and the Hessian Matrix. GAs are used for global search methods that are based on Darwin's principle of natural selection and genetic modification. GAs consists of *initial population, fitness function, selection function, crossover, and mutation*.

Therefore, based on the wider number of publications and the research done regarding GAs, it can be concluded that optimization of the suspension parameters based on the GAs platform provides suitable results, Likaj et al. [20]. The multi-objective GAs optimization method is employed for optimization of passive suspension parameters such as spring stiffness, damping coefficient, tire stiffness, sprung and un-sprung masses of the terrain vehicle.

6. Conclusion

During the modeling process of suspension system, the researchers have to make several attempts in order to be sure that the simulation results are suitable and accurate. By designing a completely new suspension mechanism which was derived by improving a double wishbone with longer equal control arms. Mathematical modeling and solving of equations of motion had been developed by numerical methods for a quarter of it. In order to provide less lateral wheel motion, the Finite Element Methods were employed in order to optimize. The proposed suspension design provides relatively small lateral wheel motion, zero camber

angles, and effectively absorbs the vibrations caused by ground excitation.

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MARINE SLOW SPEED TWO-STROKE DIESEL ENGINE - NUMERICAL ANALYSIS OF EFFICIENCIES AND IMPORTANT OPERATING PARAMETERS

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Abstract: This paper presents numerical analysis of efficiencies and non-measured operating parameters for the marine two-stroke slow speed turbocharged diesel engine 6S50MC MAN B&W with direct fuel injection. Numerical analysis was based on a measurement set performed at different engine loads. Calculated efficiencies were mechanical, indicated and effective efficiency, while the calculated important operating parameters were power of engine mechanical losses, mean effective pressure, effective engine torque and specific effective fuel consumption. Engine load was presented in percentage of maximum continuous rating (MCR). The highest engine mechanical efficiency of 94.52 % was obtained at the highest engine load, while the highest engine effective efficiency of 49.34 % was obtained at the engine load 75 % of MCR. Available engine effective torque was from 267380 Nm on the lowest up to 643594 Nm on the highest engine load, while effective fuel consumption was between 171.18 g/kWh and 186.83 g/kWh.

Keywords: MARINE DIESEL ENGINE, TWO-STROKE PROCESS, EFFICIENCIES, OPERATING PARAMETER ANALYSIS

1. Introduction

Experimental measurements are the basis of internal combustion engines operating parameters analysis [1], regardless of the engine type. By using several engine measured variables can be obtained a complete insight into engine general operating parameters, in a wide load range [2]. Numerous researchers are involved in the investigation of the diesel engines from the several points of view [3].

Marine slow speed two-stroke diesel engines, compared to the other diesel engines, are characterized by their construction, dimensions, operating processes and start-up process. Because of the high pressures and temperatures, the materials used in such engines for a large number of engine components, cannot be conventional ones [4].

Several researchers were involved in the development of numerical models for marine two-stroke diesel engines [5], in order to predict their operating parameters during the propulsion [6] or to get an insight into the details of in-cylinder processes [7] such as convective heat transfer [8].

Marine two-stroke diesel engines are turbocharged engines and it is interesting to investigate turbocharging process and its influence on engine performance [9].

To improve marine two-stroke diesel engine operating parameters and reduce emissions, numerous investigations were performed in order to implement alternative fuel combustion [10], using bio-fuel blends for combustion [11] or using standard diesel fuels with some additives [12] in this type of engines.

For this type of diesel engines were also investigated some of the known techniques from automotive diesel engines for reducing nitrogen oxides (NO_x) emissions, as for example Exhaust Gas Recirculation (EGR) [13]. It is also important to know maximum NO_x reduction potential of two-stroke marine diesel engines [14] by using EGR. Along with nitrogen oxides, for marine slow speed two-stroke diesel engines was also investigated soot emission [15] and possibilities of soot emission reduction.

This paper presents change in efficiencies and the main operating parameters of marine slow speed two-stroke diesel engine 6S50MC MAN B&W. Operating parameters and efficiency analysis was based on a measurement set performed at different engine loads (from the lowest to the highest load). For each engine operation point, by using measured parameters, was performed calculation of mechanical losses power, mean effective engine pressure, engine effective torque and engine specific effective fuel consumption. On this way was gained an insight into the change of these engine operating parameters during the whole range of observed loads. Calculated engine efficiencies and their change during the change in engine load were engine mechanical efficiency, engine indicated efficiency and on the end engine effective efficiency. This analysis confirmed that marine slow speed two-stroke diesel engines are the internal combustion engines with the highest effective efficiency

and the lowest specific effective fuel consumption, during the complete load range.

2. Slow speed marine diesel engine specifications

Analyzed marine diesel engine is a slow speed turbocharged two-stroke engine with direct fuel injection 6S50MC MAN B&W. The main engine specifications are presented in Table 1.

Table 1. Specifications of marine slow speed two-stroke diesel engine 6S50MC MAN B&W [16]

Number of cylinders	6 in line
Cylinder bore	500 mm
Cylinder stroke	1910 mm
Firing order	1-5-3-4-2-6
Maximum continuous rating (MCR)	8580 kW
Engine speed at MCR	127 rpm
Maximum mean effective pressure	18 bar
Maximum combustion pressure	143 bar
Compression ratio	17.2
Crank mechanism ratio	0.436
Exhaust manifold volume	6.13 m ³
Inlet manifold volume (with intercooler)	7.179 m ³
Cumulative engine mass	232000 kg

A cross section of the analyzed marine diesel engine 6S50MC MAN B&W is presented in Fig.1. In Fig.1 can be seen all of the housing and cylinder main elements. The engine was built in a diesel engine factory in Split, Croatia, according to the license MAN B&W.

3. Engine measurement results

The main operating data of the marine diesel engine 6S50MC MAN B&W were obtained by test-bed measurements in Shipyard Split, Croatia. Engine load was presented in percentage of maximum continuous rating (MCR), Table 1. The measured values for the engine steady state operation at engine loads 25 %, 50 %, 75 %, 93.50 % and 100 % of MCR was presented in Table 2.

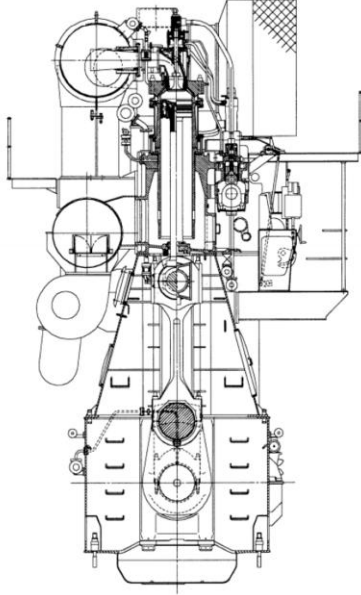


Fig.1. Cross section of marine slow speed two-stroke diesel engine 6S50MC MAN B&W [17]

Table 2. 6S50MC MAN B&W measured data [16]

Load (% of MCR)	Indicated power (kW)	Effective power (kW)	Mean indicated pressure (bar)	Rotational speed (rpm)	Fuel mass flow (kg/h)
25 %	2401	2142	8.37	76.5	400.2
50 %	4406	4099	12.24	96.0	713.5
75 %	6580	6160	15.89	110.4	1054.5
93.50 %	8170	7667	18.38	118.5	1317.3
100 %	8656	8182	19.01	121.4	1429.1

The measurements were performed during the following environmental conditions:

- Ambient temperature 30 °C,
- Ambient pressure 1005 mbar,
- Relative humidity 50 %.

The engine was tested with a standard marine diesel fuel, whose properties are:

- Density 844.7 kg/m³,
- Kinematic viscosity 3.03 mm²/s,
- Sulfur content 0.45 %,
- Lower heating value 42625 kJ/kg.

4. Equations for calculating engine efficiencies and operating parameters

Power of mechanical losses for each operating point of the analyzed engine should be calculated as a difference between measured indicated and effective power, Table 2:

$$P_{ml} = P_{ind} - P_{eff} \quad (1)$$

where P_{ml} (kW) is power of mechanical losses, P_{ind} (kW) is measured indicated power and P_{eff} (kW) is measured effective power.

Engine mechanical efficiency was calculated by using an equation:

$$\eta_m = \frac{P_{eff}}{P_{ind}} \cdot 100 \quad (2)$$

where η_m (%) is engine mechanical efficiency.

Indicated engine efficiency is the ratio of engine indicated power and heat released by fuel. Indicated engine efficiency was calculated according to the equation:

$$\eta_{ind} = \frac{P_{ind}}{\dot{m}_f \cdot H_{low}} \cdot 3600 \cdot 100 \quad (3)$$

where η_{ind} (%) is engine indicated efficiency, $\dot{m}_f$ (kg/h) is measured fuel mass flow - Table 2 and H_{low} (kJ/kg) is used fuel lower heating value.

Effective engine efficiency is the ratio of engine effective power and heat released by fuel. Effective engine efficiency was calculated according to the equation:

$$\eta_{eff} = \frac{P_{eff}}{\dot{m}_f \cdot H_{low}} \cdot 3600 \cdot 100 \quad (4)$$

where η_{eff} (%) is engine effective efficiency.

Engine mean effective pressure was calculated by using an equation:

$$p_{me,eff} = \frac{P_{eff} \cdot \tau}{2 \cdot z \cdot n \cdot V_{op}} \cdot \frac{6}{10} \quad (5)$$

where $p_{me,eff}$ (bar) is engine mean effective pressure, τ (-) is engine stroke - analyzed engine is two-stroke engine so $\tau = 2$, z (-) is number of engine cylinders - Table 1, n (rpm) is measured engine rotational speed - Table 2 and V_{op} (m³) is operating volume of one engine cylinder which can be calculated according to the equation:

$$V_{op} = \frac{D^2 \cdot \pi \cdot s}{4} \quad (6)$$

where D (m) is cylinder bore - Table 1 and s (m) is cylinder stroke - Table 1.

Engine effective torque, which drives the ship's propeller was calculated according to the equation:

$$M_{eff} = \frac{P_{eff}}{2 \cdot \pi \cdot n} \cdot 60000 \quad (7)$$

where M_{eff} (Nm) is engine effective torque.

Specific effective fuel consumption was calculated by using an equation:

$$b_{eff} = \frac{\dot{m}_f \cdot 1000}{P_{eff}} \quad (8)$$

where b_{eff} (g/kWh) is engine specific effective fuel consumption.

5. Engine calculation results for various observed loads and discussion

Fig.2 presents the power of mechanical losses calculated by using equation (1) and mechanical efficiency calculated by using equation (2) for all observed loads of the analyzed engine.

Engine power of mechanical losses is the lowest at load 25 % of MCR and amounts 259 kW, while the highest power of mechanical losses can be seen at load 93.5 % of MCR where it amounts 503 kW. At the highest engine load 100 % of MCR, power of mechanical losses decrease from the highest value and amounts 474 kW.

The mechanical efficiency of the analyzed engine continuously increases during the increase in engine load. At the lower engine load 25 % of MCR, mechanical efficiency is the lowest and

amounts 89.21 %, while on the highest engine load 100 % of MCR mechanical efficiency of the engine is the highest and amounts 94.52 %. This is an important fact, because for the analyzed engine it can be expected that the majority of its operation will be obtained at the highest load. Therefore, during the majority of engine operation, mechanical efficiency will be the highest.

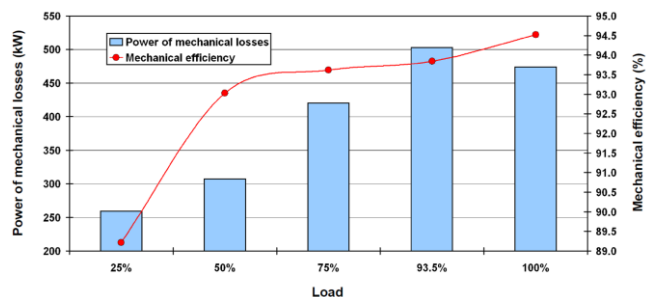


Fig.2. Change in engine power of mechanical losses and mechanical efficiency for all observed loads

Analyzed engine indicated efficiency change, calculated according to equation (3) and engine effective efficiency change, calculated according to equation (4) are presented in Fig.3. From the lowest to the highest engine load, both efficiencies have the same trend - they increase until the engine load 75% of MCR after which both of them decreases.

Indicated engine efficiency is the ratio of the engine indicated power and heat released by fuel, so this efficiency presented amount of energy which is transferred from fuel to the engine pistons. At the lowest engine load 25 % of MCR indicated efficiency is the lowest and amounts 50.67 %. Increase in engine load firstly causes an increase of indicated efficiency to a maximum value of 52.70 % at the engine load 75 % of MCR after which follows a decrease in indicated efficiency to 52.38 % (engine load 93.50 % of MCR) and to 51.16 % (engine load 100 % of MCR).

Engine effective efficiency has the lowest value of 45.21 % at the engine load 25% of MCR while the highest effective efficiency amounts 49.34 % at the engine load 75 % of MCR. At the highest engine load 100 % of MCR, effective efficiency amounts 48.36 %. In comparison with all the other types of internal combustion engines, marine slow speed two-stroke diesel engine has significantly higher effective efficiency, which can nowadays reach above 50 % (maximal obtained effective efficiency of marine two-stroke diesel engine is 55 %). Effective efficiency of analyzed diesel engine does not reach 50 % for any observed load, but is very close to that value.

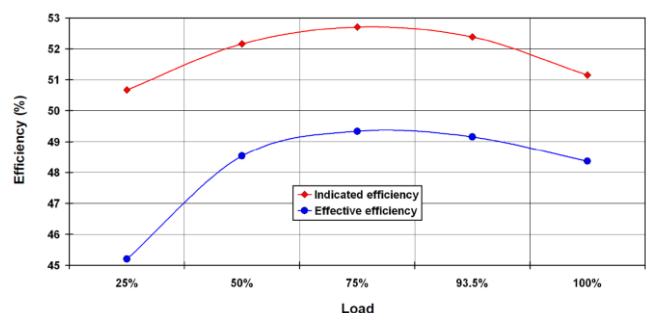


Fig.3. Change in engine indicated and effective efficiency for all observed loads

The change in mean effective pressure of the analyzed engine, for all of the observed engine loads was presented in Fig.4. Mean effective engine pressure was calculated according to equation (5) and in Fig.4 was presented along with measured mean indicated engine pressure.

During the increase in engine load, mean effective pressure continuously increases from 7.47 bar at the engine load 25 % of

MCR up to 17.97 bar at the engine load 100 % of MCR. At the maximum engine load 100 % of MCR was obtained almost the maximum mean effective pressure, which amounts exactly 18 bar, Table 1.

Measured indicated and calculated effective pressures of the analyzed engine have the same trends during the increase in engine load from the lowest to the highest loads.

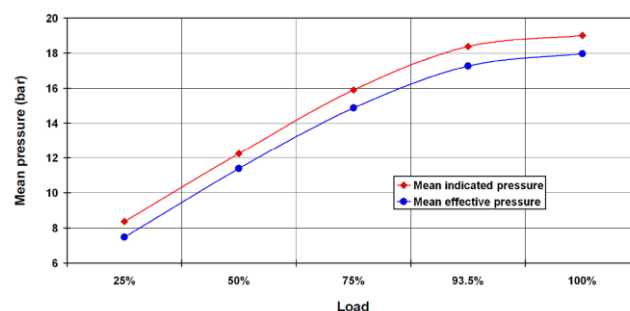


Fig.4. Change in engine mean indicated and effective pressure for all observed loads

Engine effective torque, calculated by using equation (7) continuously increases during the increase in engine load, Fig.5. In comparison to other diesel engines, marine slow speed two-stroke diesel engines develop significantly higher engine effective torque which will be used for propulsion propeller drive. One of slow speed marine diesel engine advantages is direct propeller drive, without usage of gearbox, so the developed effective torque was directly transferred to the main ship propeller.

The lowest effective torque analyzed engine develops on the lowest observed load 25 % of MCR, and that effective torque amounts 267380 Nm. On the highest observed engine load 100 % of MCR was developed the highest engine effective torque which amounts 643594 Nm. For marine two-stroke diesel engine, with cylinder bore of 500 mm, this is an expected range of developed effective torque. The highest developed effective torque must be obtained at the highest engine load, because at the highest engine load can be expected the majority of ship operation (maximum ship speed).

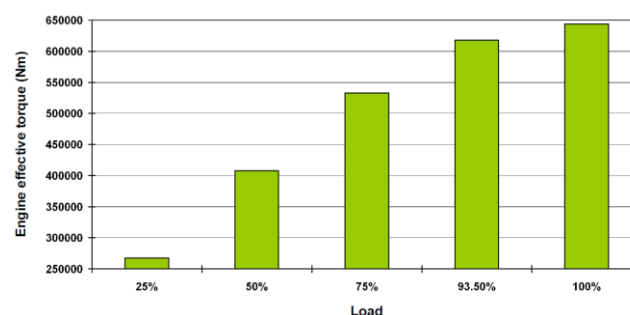


Fig.5. Change in engine effective torque for all observed loads

When compared specific effective fuel consumption of the analyzed engine with other diesel engines, for example, with a high speed direct injection turbocharged diesel engine MAN D0826 LOH15 presented in [18], it can be calculated that marine two-stroke diesel engine has much lower specific effective fuel consumption. This is not a fact only for two compared diesel engines, marine two-stroke diesel engines have the lowest specific effective fuel consumption of all diesel engines or of all engines in general. This fact is valid if compared diesel engines which use standard diesel fuel, if diesel engine use the alternative fuels, this conclusion does not have to be correct.

Specific effective fuel consumption of the analyzed engine, calculated by using equation (8), has the same trend like the other diesel engines - during the load increase specific effective fuel consumption firstly decrease to the lowest value, after which

follows slight increase, Fig.6. The highest specific effective fuel consumption of the analyzed engine was obtained at the lowest load 25 % of MCR and amounts 186.83 g/kWh. Increase in engine load causes that specific effective fuel consumption decreases and the lowest value were obtained at the engine load 75 % of MCR and amounts 171.18 g/kWh. A further increase in engine load causes an increase in specific effective fuel consumption and at the highest engine load 100 % of MCR specific effective fuel consumption of the analyzed engine amounts 174.66 g/kWh.

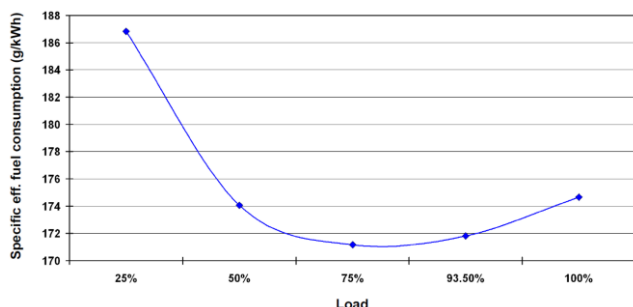


Fig.6. Change in engine specific effective fuel consumption for all observed loads

6. Conclusion

Calculated operating parameters and efficiencies of marine slow speed two-stroke diesel engine 6S50MC MAN B&W was analyzed in this paper. Analysis was based on a measurement set performed at different engine loads in order to obtain complete range of main engine parameters and efficiencies change.

Presented calculation method gives for result that the highest engine mechanical efficiency of 94.52 % was obtained at engine load 100 % of MCR. The highest indicated engine efficiency of 52.70 % and the highest engine effective efficiency of 49.34 % were obtained at the engine load 75 % of MCR. In comparison with the other types of internal combustion engines, marine slow speed two-stroke diesel engines have significantly higher effective efficiency which can nowadays reach above 50 %.

The highest power of engine mechanical losses was obtained at engine load 93.50 % of MCR and amounts 503 kW. During the engine load increase, mean effective pressure continuously increases from 7.47 bar at the lowest up to 17.97 bar at the highest observed engine load. The range of available engine effective torque was from 267380 Nm on the lowest up to 643594 Nm on the highest engine load, what is an expected range of developed effective torque for this kind of diesel engine.

The range of analyzed engine specific effective fuel consumption was between 171.18 g/kWh and 186.83 g/kWh. Obtained range of specific effective fuel consumption proves the fact that marine two-stroke diesel engines have the lowest specific effective fuel consumption of all diesel engines or of all engines in general.

7. Acknowledgments

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MULTILEVEL MODIFICATION IN MATERIALS SCIENCE AND POLYMER NANOCOMPOSITES TECHNOLOGY

МНОГОУРОВНЕВОЕ МОДИФИЦИРОВАНИЕ В МАТЕРИАЛОВЕДЕНИИ И ТЕХНОЛОГИИ ПОЛИМЕРНЫХ НАНОКОМПОЗИТОВ

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Abstract: This paper describes directions of realization of the multilevel modification principle in materials science and technology of polymer composite materials based on thermoplastics. It is shown that the introduction of nanoscale particles of different structures and production technologies into the composition of the composite makes it possible to transform the structure at various organization levels, which leads to the achievement of a synergistic effect of increasing the parameters of deformation-strength, tribotechnical characteristics and resistance to the action of thermal-oxidative medium. One of the perspective technologies of the nanomodifiers introduction into the composite material is the diffusion treatment of components and products in precursor solutions. Mixture of composite materials with increased parameters of performance characteristics for use in engineering, chemical and mineral resource industries have been developed.

KEYWORDS: MULTILEVEL MODIFICATION, NANOMODIFIER, NANOCOMPOSITE, POLYMER BLENDS, POLYMER STABILIZATION

1. Introduction

Review of recent results [1 – 7] in materials science and technology of polymeric functional materials area allows us to assert about the prevalence of the structural factor in the achievement of the set value of stress-strain, tribotechnical adhesion, and other characteristics of products under different operating factors intensity. Traditional methodology of polymer materials creation for the production of components for static (adhesive) and dynamic (tribotechnical) metal-polymer systems with various functionality and operating conditions is based primarily on methods of managing a structural organization that take into account the influence of one or several prevailing factors – thermophysical, deformation, corrosive, destructive, etc. [1, 3 – 12]. The practical realization this methodology is based on managing the structural parameters of composites at one of the levels of their organization (molecular, intermolecular, supramolecular and interphase) by introducing of functional components into the composition of the material or using special methods for modification of products (Fig. 1). A system approach to determining the potentialities of composite materials to adequately counteract the operational factors that cause the destruction or wear of the components of the metal-polymer system indicates the necessity to take into account the combined effect of various physical and chemical, thermal, deformation, corrosion, electrophysical and other processes that determine the mechanisms and kinetics of structural transformations at various organizational levels. The prospective of the system approach has been proved in a number of studies devoted to the development of low-wearing metal-polymer systems by introducing components that form a structure with the function of inhibitors of unfavorable processes under the influence of operational factors [13].

It is obvious that the new generation composite materials should transform the original structure with a high degree of adequacy under the influence of variable operational factors with varying intensity for optimal confrontation and preservation of the specified parameters for safe, efficient and comfortable operation of the metal-polymer system of a certain design and functionality. In this regard, the development of technological methods for practical implementation of the principle of multilevel modification [14] has a special perspective.

2. Research methods

For research we used polymer materials belonging to the class of aliphatic polyamides: PA6, PA6.6 (Branch “Khimvolokno Plant” of

Public Joint-Stock Company “Grodno Azot”, Belarus), PA66/6 Grilon TSS/4, PA12 Grilamid L20 (EMS-CHEMIE AG, Switzerland), PA11 Rilsan (Arkema, France). Some experiments were carried out with polyolefins – polypropylene (PP), low-density polyethylene (LDPE) and high-density polyethylene (HDPE).

For control the parameters of the structure and performance characteristics of composite materials we used dispersed (including nano-sized) carbon-containing particles (colloidal graphite preparation C-1, detonation synthesis ultradispersed diamonds (UDD) (Scientific and Production Closed Joint-Stock Company “SINTA”, Belarus), carbon nanotubes (CNTs) (A. V. Luikov Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus)), silicon-containing (clays, tripoli) and metal-containing (copper formate) compounds obtained by original technologies of producers.

The components were combined by extrusion blending technology on a twin screw extruder of compounding line Berstorff Compex MPC 67/2, thermomechanical mixing in the material cylinder of the injection molding machine Battenfeld TM (Wittmann Battenfeld GmbH, Germany) under the conditions specified by the equipment manufacturers.

Diffusion modification of granular or powder semi-processed polymer materials was carried out by exposure in a precursor solution (copper formate) for 1 to 10 hours with drying for removing of the solvent.

Physical and chemical processes at various levels of the structural organization of composite materials were investigated by using modern methods of analysis: IR spectroscopy (Tensor-27), X-ray diffractometry (Dron-3.0), differential thermal analysis (Thermoscan-3), atomic-force (AFM), scanning electron (SEM) and optical microscopy by the instrumentality of devices Mira, Tescan, NT-206, MDS.

The parameters of stress-strain, tribotechnical and adhesion characteristics of composite materials and coatings were evaluated according to standard methods by using specialized equipment – tensile-testing machine Z010 Zwick and tribo-test device FT-2. The results were processed using the software products included in the equipment package. Data processing were carry out by using software of current technique.

3. Results and discussions

In various metal-polymer constructions the composite materials are exposed by prolonged exposure of higher temperatures which intensify the processes of thermal-oxidative degradation leading to the reduction of parameters of stress-strain, tribological, adhesive

and other characteristics [1, 3 – 8, 13, 14]. The increase of the polymer and composite materials products resistance to aging under

the influence of operational factors is one of the topical problems of functional materials science [13].

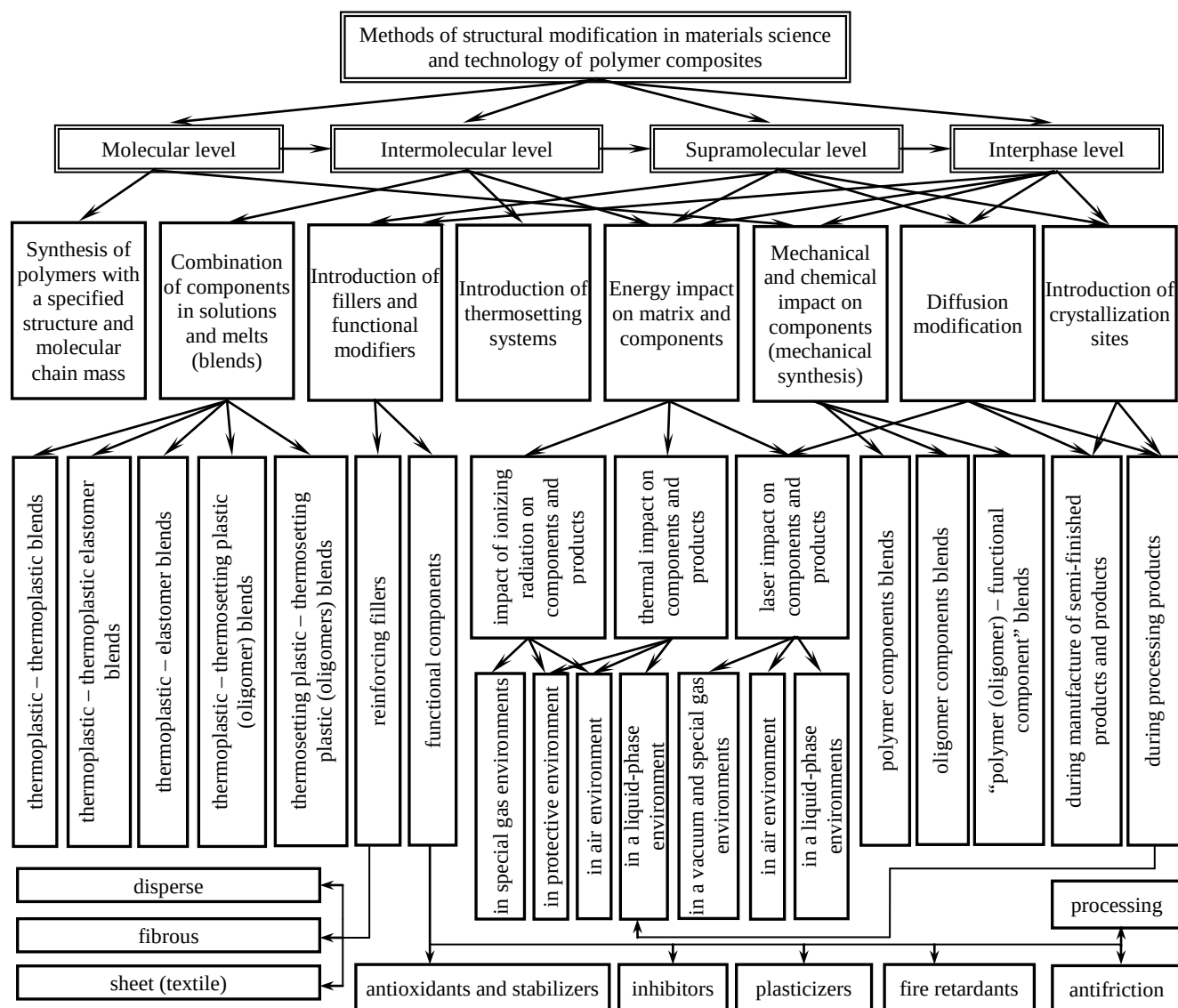


Figure 1 – The main directions of structural modification in materials science and technology of polymer composite materials

An effective direction of the increase of the polymer and composite materials products resistance to thermal-oxidative aging is the realization of the mechanism of non-chain stabilization proposed in the works of Gladyshev G. P. and co-workers [18]. The essence of this mechanism consists in introducing into the composition of components capable of preferentially interacting with active oxygen to form oxide compounds. At the same time, the chain processes of thermal oxidation and destruction of the matrix binder are inhibited. It has a positive effect on the resistance of the products. As such “nonchain” stabilizers, the highly dispersed metal particles with a high sensitivity to oxygen are effective. The approaches proposed in [18] are based on the mechanisms for preventing or reducing the probability of interaction of oxygen atoms (ozone) with the active sites of the macromolecules of the binder and are realized when there are sufficient amounts of modifiers with increased affinity for oxygen in the composite. After the exhaustion of the active modifier, the intensity of the processes of thermal-oxidative degradation and aging increases. It leads to a decrease of the service life of products.

An effective direction of realization of the mechanism of nonchain stabilization in polymer composites based on

thermoplastics is the introduction of nanoscale metal particles by thermolysis of metal-containing precursors directly in the melt of the matrix binder during the processing of the composite into a product by injection molding or extrusion [13, 14]. This approach, based on the classical ideas of the influence of supermolecular structure on the kinetics of thermal-oxidative and thermodestruction processes in thermoplastics worked out by prof. Maciulis A. N. [19], was developed in the studies of prof. Struk V. A., prof. Ryskulov A. A. and them colleagues [13, 20, 21]. A special mechanism for the non-chain stabilization of thermoplastic polymers of a class of polyamides, polyacetals, polyolefines and their thermomechanically combined mixtures containing nanoscale metal particles was established. This mechanism consists of a combination of structural factors and phase transformations in metal-polymer composites with a doping content (0.01 – 0.5 wt. %) of a modifier. An important result of the carried out complex studies is the established fact of the change in the energy parameters of the macromolecule of the matrix polymer as a result of the interaction of their active sites with the nanoscale particles of the modifiers (particles of metals and oxides) formed during the thermolysis of the metal precursor.

We made an assumption, that it is possible to realize the mechanism of nonchain stabilization like in metal-polymer systems [21] for composites containing other (including nonmetallic) modifiers with a nanoscale range of the particles.

For research we have chosen aliphatic polyamides and nanosized carbon-containing particles – carbon nanotubes (CNTs), detonation synthesis ultradispersed diamonds (UDD), colloidal graphite preparation C-1 (CGP C-1) in the state of industrial supply.

For evaluation of the effectiveness of nanosized carbon-containing particles action we have used model composites based on aliphatic polyamides PA6, PA6.6, PA11, PA12, containing nanosize copper particles with a content of 0.075 – 0.6 wt. %. The nanoscale metal-containing modifier was obtained by heat treatment of granular or powder semi-finished products diffusively modified in aqueous solutions of a metal precursor (copper formate) for 1 to 10 hours.

A comparative evaluation of the effectiveness of nanodimensional modifiers in original, mixed and composite polyamide matrices was carried out according to the parameters of stress-strain characteristics of standard samples exposed to thermal-oxidative aging at a temperature of 423 ± 5 K (150 ± 5 °C) in air for 200 hours. As a criterion, the tensile strength σ , MPa was chosen. Experimental data are given in Figures 2 and 3.

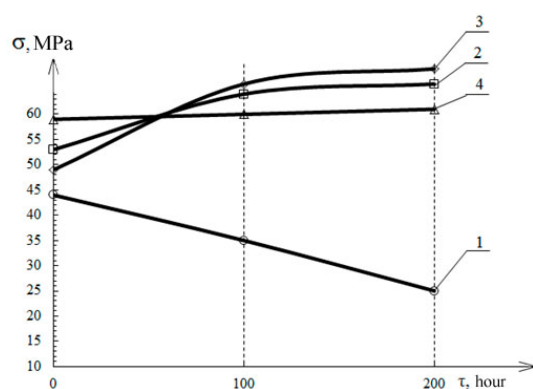


Figure 2 – The graph of relationship of tensile strength σ to heat treatment time τ at 423 K (150 °C) for PA6 (1), PA6 + copper formate (after 1 hour of diffusion modification) (3), PA6 + copper formate (after 5 hours of diffusion modification) (2), PA6 + copper formate (after 10 hours of diffusion modification) (4)

As follows from the data presented in Fig. 2, the diffusion treatment of granulated polyamide 6 (PA6) in an aqueous solution of copper formate $[\text{Cu}(\text{HCOO})_2]$ for 1–10 hours leads to a significant change in the resistance of standard samples to thermal-oxidative aging. The original tensile strength parameter of samples from PA6 decreases from 44.67 MPa to 26.66 MPa after 200 hours of thermal oxidation in the air medium (Fig. 2 curve 1). At the same time, the samples modified by nanoparticles of copper not only do not reduce the original tensile strength parameter, but also significantly increase it to 61.95–67.22 MPa after thermal oxidation for 100–200 hours (Fig. 2 curves 2, 3, 4).

The obtained results confirm the basic positions of the mechanism of action of nanoscale copper particles, described in [13]. It should be noted that the diffusion mechanism of introducing nanoscale particles into the polymer matrix has a special perspective of practical application, because it is characterized by the simplicity and availability of technical operations to achieve a technically significant effect in comparison with other technologies, for example, blending or mixing.

A similar technically significant effect of increasing the resistance to thermal-oxidative aging has been achieved for samples of composite materials based on polyamide PA6 modified by fire-retardant agents (PA6-GF) and a combination of fire-retardant agents with 20 wt. % fiberglass (PA6-FG20-GF). The introduction of nanosized copper particles into the composites in the amount of 0.085 – 0.6 wt. % by diffusion treatment in an aqueous solution of

copper formate significantly increases not only the original parameters of stress-strain characteristics, but also their values after 100 hours and 200 hours of thermal oxidation at a temperature of 423 ± 5 K (Fig. 3).

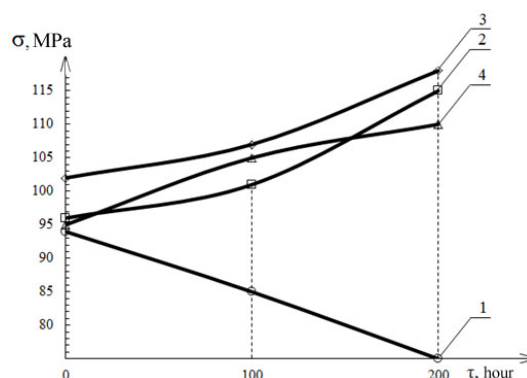


Figure 3 – The graph of influence of nanoscale copper particles on the resistance of glass-filled polyamide to thermal-oxidative degradation for PA6-FG20-GF (1), PA6-FG20-GF + copper formate (after 1 hour of diffusion modification) (2), PA6-FG20-GF + copper formate (after 5 hours of diffusion modification) (3), PA6-FG20-GF + copper formate (after 10 hours of diffusion modification) (4)

A significant increase of the tensile strength parameter for composites PA6-GF modified by copper nanoparticles indicates the realization of structural modification mechanisms at various levels, proposed in [13, 14].

For composites containing functional filler (fire-retardant agents and fiberglass) the structuring effect is observed when copper nanoparticles are introduced. This effect is manifested in a decrease of deformation evaluated by the tensile elongation criterion.

The most important factor of increasing the resistance of carbon-containing nanocomposites based on combined aliphatic polyamides to thermal-oxidative aging is the structure formed by close-structure macromolecules at different levels – intermolecular, supramolecular and interphase.

It is known that aliphatic polyamides are partially crystalline polymers with predominantly spherulite type of supramolecular structure [19].

As shown in the studies of prof. Savkin V. G. and co-workers [15] in the realization of the increased parameters of the stress-strain characteristics of polyamides, the dimensions of the spherulites, their structural perfection and the parameters of the spherulite interface are most important.

Due to the close structure of the macromolecules of the matrix polyamide PA6.6 and the modifiers PA6, PA12, the spherulite structure of the blend composite is formed with the participation of pass-through macromolecules. As a result, there is formation of a structure similar to the cross-linked, created by the pass-through macromolecules of the alloying polyamide. Such a structure is able to withstand the action of external loads applied to the sample (product). In addition, the presence of a low-melting component (PA12) in the composite promotes to reduce residual stresses during crystallization and chilling of the matrix polymer (PA6.6).

These factors contribute not only to a significant increase of the parameters of stress-strain characteristics of blend composites, but also to resistance to thermal-oxidative medium. In this case, the tensile strength parameter significantly decreases.

When nanodispersed carbon-containing particles, mainly located in the interspherulite regions, are introduced into the blend composite, the effect of higher resistance to thermal-oxidative degradation increases due to the formation of additional physical bonds of the adsorption type (Fig. 4).

Thus, nanosized carbon-containing particles act as a physical compatibilizer. It is stimulate to the formation of a perfect composite structure at different levels of organization.

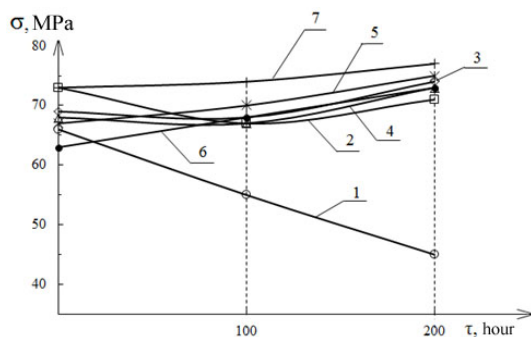


Figure 4 – The graph of relationship of tensile strength σ to heat treatment time τ at 423 K for polyamide composite materials:

- 1 – PA 6.6;
- 2 – PA6.6 (94 wt. %) + PA6 (5 wt. %) + PA12 (1 wt. %);
- 3 – PA6.6 (90 wt. %) + PA6 (5 wt. %) + PA12 (5 wt. %);
- 4 – PA6.6 (85 wt. %) + PA6 (10 wt. %) + PA12 (5 wt. %);
- 5 – PA6.6 (84.5 wt. %) + PA6 (10 wt. %) + PA12 (5 wt. %) + CGP C-1 (0.5 wt. %);
- 6 – PA6.6 (84.5 wt. %) + PA6 (10 wt. %) + PA12 (5 wt. %) + CNT (0.5 wt. %);
- 7 – PA6.6 (84.5 wt. %) + PA6 (10 wt. %) + PA12 (5 wt. %) + UDD (0.5 wt. %)

Thus, the modification of blend composites based on aliphatic polyamides with nanoscale particles with different structure and production technology makes it possible to realize the synergistic effect of increasing the parameters of stress-strain, adhesion, tribotechnical characteristics and resistance to the action of thermal-oxidative operating media. The mechanism of synergistic effect realization is due to the interaction of active sites of nanosized particles with the sites of polymeric macromolecules with the formation of adsorption type bonds [14]. The formation of such bonds changes the intensity of intermolecular interaction in composites based on mono- and blend matrices. It is manifested in the transformation of the structure of the composite at the intermolecular, supramolecular and interphase levels. Due to the multilevel structural modification, the resistance to influence of operational factors (including to the processes of tribochemical interaction in metal-polymer systems and high temperatures in the air environment) is increases.

The effect of the antioxidant effect of nanoscale carbon-containing particles of different structures and synthesis technology is mainly due to the adsorption interaction of active sites with the formation of physical bonds. This hypothesis is confirmed by the facts of changes not only parameters of thermophysical characteristics during introducing doping amounts of the modifier (0.01–1.0 wt. %), but also of rheological and stress-strain properties. At the doping content of a nanosized modifier the amount of carbon-chain compounds that can perform the function of the antioxidant of polymer matrix, as noted in [22], is insignificant and can not have any significant effect on the kinetics of thermo-oxidative processes during long exposure times in an oxidizing environment. Therefore, the prevailing role in the demonstration of the antioxidant effect belong to reduce the sensitivity to oxygen by macromolecular due to a decrease their activity determined by the formation of physical spatial bonds. Thus and so, this effect is relevant for different nanosize particles, which do not belong to antioxidants in the common sense of the term. It is confirmed by the smooth behavior of experimental curves $\sigma = f(\tau)$ for the nanocomposites at the time of thermal oxidation up to 1000 hours as opposed to the analogous experimental curves typical for composites containing antioxidants (these curves characterized by a spasmodic change in the parameter σ after the consumption of the antioxidant) [19].

A special perspective in the realization of the principle of multilevel modification in composite materials based on

thermoplastic blends is the technology of introducing nanoscale particles by diffusion of solutions of various compounds.

In the case of diffusion modification of composite products based on blend matrices or reinforced by fragments of carbon, glass and other fibers, the effect of structural modification of the most defective structureless layer is realized. This layer largely determines the performance parameters of metal-polymer systems, primarily adhesion and tribotechnical characteristics. A sufficiently large thickness of the diffusion-modified layer [19] makes it possible to realize the gradient structure of the product. The near-surface layer of this product is a nanocomposite material with a high degree of structuring. It due to the formation of a spatial grid of adsorption physical bonds determined by the localization of nanoparticles in intermolecular regions and structural defects. The nanostructured layer is located on a composite base formed by a matrix binder and functional components with various functionality. During the introducing of reinforcing fibers into a composite, their functions are realized increasingly due to the formation of a nanostructured near-surface layer and a decrease of the probability of formation and development of microcracks under the action of mechanical, thermal, thermomechanical stresses arising under the operational factors.

The combination of various techniques of introducing nanoscale particles into the composite material, for example, diffusion treatment of the granules of the components (filled and unfilled) and the product obtained from these granules, makes it possible to form a composite structure with optimal organization at various levels. Such a structure forms prerequisites for the realization of synergistic effects in various mechanisms of their demonstration. For example, as shown before, in the blends based on thermoplastic components or composite materials containing functional components, along with the achievement of increased parameters of stress-strain, adhesion and tribotechnical characteristics, we have a technically significant effect of increasing the resistance to thermal-oxidative aging. This effect, in some cases, determines the parameters of the service life and reliability of the metal-polymer system. It should be emphasized that the effect of increasing the resistance to the action of thermal-oxidative medium is manifested not only in the diffusion introduction of antioxidants [19], but also in the diffusion introduction of nanoscale particles with different nature and structure.

4. Conclusions

The methodology of realization the principle of multilevel modification for the creation of metal-polymer systems components with high parameters of performance characteristics is considered. It is shown that, for composites based on polyamides containing functional components (reinforcing fibers, flame retardants), it is advisable to introduce nanosize particles by preliminary diffusion treatment of granulated semi-finished products in aqueous solutions of thermally decomposing precursors. On application of this technology, a synergistic effect of increasing the parameters of combustion resistance and the resistance of materials to the action of thermo-oxidative medium is realized. At the same time, high values of parameters of stress-strain characteristics are maintained.

For composites obtained by thermomechanical combination of aliphatic polyamides with different structure and molecular chain mass, it is effective to introduce the nanosized carbonaceous particles (colloidal graphite preparation C-1, carbon nanotubes, UDD), which contribute to the formation of a structure providing high parameters of performance characteristics (adhesion, tribotechnical, stress-strain) with simultaneous increase of resistance to thermal-oxidative aging. Additional modification of semi-finished products (granules or powders) by copper formate with using the diffusion treatment contributes to the increase of the parameters of the performance characteristics.

A mechanism for realizing the principle of multilevel modification in filled and blend composites is proposed. This mechanism consists in the formation of an optimal structure at different levels of organization – intermolecular, supramolecular

and interphase, due to the formation of a spatial grid of adsorption physical bonds between nanoparticles and active sites of polymeric macromolecules. The presence of such bonds in combination with the functional action of the components introduced into the composite creates the prerequisites for the realization of the synergistic effect of increasing the values of the performance parameters.

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DETERMINING OF STORAGE SITE LOCATION WITHIN PRODUCTION SYSTEMS

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Abstract: Analysing of material flows within the boundaries of the production system it is possible to conclude that the sources and sinks of those material flows are storages. In those storages in the function of the kind and the type numerous processes are implemented. These storage processes along with the material handling processes are responsible for quantitative and dynamic balancing of material flows and as such have a significant impact on the total cost and productivity of the production system. Due to the above reasons, the design of storage is an important task which needs to be adequately accessed. Regardless of the kind and the type and the associated processes within storage one of the main activities in the design phase of storage is to define its location, with special emphasis on interaction with other elements of the production system (production and processing equipment, material handling equipment and devices, etc.). Namely, selection of the right location, among other things ensuring the necessary conditions which will make the process of storage to meet the technical and technological, economic, organizational, IT and other requirements upon it.

Keywords: MATERIAL FLOW, STORAGE, MATERIAL HANDLING, PRODUCTION FACILITY, LOCATION, TRANSPORTATION COSTS, SOFTWARE SOLUTION

1. Introduction

Material flows within the production systems are the basis for realisation of manufacturing processes and they incorporates processes of movement of materials between/within the production units, and the processes associated with the "inaction" of the transportation units within the limitations of the considered production system. Regardless of the type of activities that are realized in particular case, costs associated with material flows represent additional costs which, if not adequately observed and treated, result in an increasing of total production costs and a reduction in the competitiveness of the production system.

Activities associated with the "inaction" of transportation units within the production systems are in most cases recognized as storage processes and include all the activities for which the transportation units for a longer or shorter period of time, temporarily or occasionally are bring in to idle status in the order to dynamically balance - synchronize (time, space, and quantity) of production processes within which they exist. In this case, transportation units are recognized as storage units. By realizing the storage activities, the flow of material within the production systems is interrupted or stopped, thus increasing the cost of the production process. Regardless of the reasons why the transportation units within production system is brought to a standstill – they stored, the appropriate storage space itself can be defined as a well-equipped and well-organised place within the production system that provides all the necessary conditions for disposal, storing, preparing and issuing of warehouse units before, during and after their usage within in the production process [1].

Depending on the purpose and location within the production system, it is possible to identify several types of storages: input, reception, interphase, auxiliary and exit storages. Auxiliary and interphase storages facilities are inherent to the immediate production ie they are located inside or directly alongside production capacities and from the point of view of storage processes those are short-term storages. Additionally, interphase storages has a task to realize activities related to short-term time synchronization of flows of material between different production operations, while auxiliary storages depending on the type of production are used as the:

- "issuer" of working tasks, and in accordance to the norms, standards and requirements serves for storage of handy tools, work and safety equipment, common equipment and supplies for workplaces in the individual and in small-series production;

- "feeders" of tools, materials and means for the production, documentation, spare parts, lubricants, etc. for the production lines in serial and mass production.

Given the type of tasks that are being carried out within the auxiliary and interphase storages, it is necessary to adequately consider all the tasks needs to be perform within those types of storages and in accordance with the set up requirements, respecting the minimum cost criteria, design those types of storages. One of starting steps in designing of these types of storages is the choice of storages locations within the certain production facility.

2. Methods for determining of auxiliary storage site location in production facilities

Regardless to the type and purpose of the storage space within the industrial enterprise, the choice of its location is conditioned by minimum costs and providing an adequate service to the users, for example production working places. Above mentioned is based on the balance of materials determined by the internal flow of materials and the layout of the users that requires storage services. Generally, the procedure of selection of storage site location is a systemic activity that is accomplished by applying the appropriate methods and includes [2, 3]:

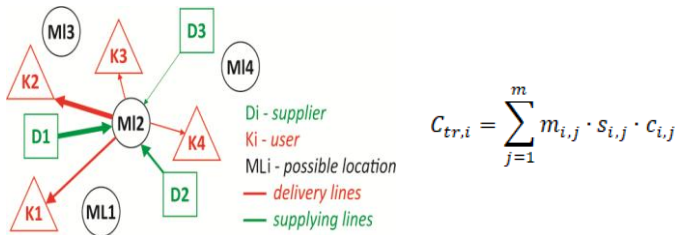
- defining of a set of influential factors relevant to the choice of storage site location;
- prediction and assessment of the intensity, direction and course of the action of identified influential factors in the given time and environmental conditions in terms of deciding on the location of storage;
- evaluation of variants of possible solutions and the selection of optimal storage site location.

Table 1: Determining of the storage site location by the method of assessment of indicators [4]

Num.	Indicators	Potential location				
		x	y	...	z	
1.	P_1	x_1	y_1	...	z_1	points
2.	P_2	x_2	y_2	...	z_2	
.	.	.	.	.	.	
.	.	.	.	.	.	
i.	P_i	x_i	y_i	...	z_i	
TOTAL:		$\sum x_i$	$\sum y_i$	...	$\sum z_i$	
SOLUTION:						
$\max \{ \sum x_i, \sum y_i, \dots, \sum z_i \}$						

During the realization of the above mentioned activities, it starts from the generally defined objectives of the production system from the point of view of the realization of the storing activities and the definition of the site location, taking into account the external and internal factors, gradually limiting the choice of the storage site location in accordance to the specific objectives and tasks set forth above. Depending on the criteria and approaches to the determining of the storage site location, several groups of methods have been developed such as: methods based on assessment of specific indicators, methods based on calculation of transportation cost, methods based on value analysis, methods based on calculation of account investment costs, etc.

Methods based on assessment of specific indicators are mainly used in the pre-selection stages of the storage site location where, based on a certain number of indicators and an adequate point evaluation of each of them on the basis of the resulting sums, an storage site location is determinate, table 1.



, where are:

$C_{tr,i}$ - overall transportation costs for specific location, [nj]
 m_{ij} - amount of transport between supplier/user j and location i , [t]
 s_{ij} - distance between supplier/user j and location i , [m]
 c_{ij} - transportation costs between supplier/user j and location i , [nj/t·m]
[nj] - money units

Fig. 1 Determining of storage site location by model of calculation of transportation costs [5]

Methods that take into account transportation costs, as their name suggests, are mostly used in cases where relatively large transportation costs are expected, i.e. when the transportation path is long. A number of methods have been developed in this group, and some of them are: *Launhardt* graphical method, *Rockstroh* method, method of „northwest angle“, etc. For the application of these methods it is necessary to know the quantity of transported material, the types of transportation equipment, the distance between the locations, etc. Based on the above data, the calculation of the transportation costs between each of the potential storage sites location and the subject that indicate the storage requirement is made. The criterion of minimum transportation costs is crucial for the selection of storage site locations, figure 1.

Table 2: Determining of the storage site location by value site analysis [4]

Table 2: Determination of the storage site location for the first location								points
Num.		Indicators		Weight coefficient w				
1.		P_1		w_1				
2.		P_2		w_2				
.		.		.				
i		P_i		w_i				
TOTAL:				100				
POTENTIAL LOCATION								
Num.	x	$w \times x$	y	$w \times y$	...	z	$w \times z$	
1.	x_1	$w_1 \times x_1$	y_1	$w_1 \times y_1$	...	z_1	$w_1 \times z_1$	
2.	x_2	$w_2 \times x_2$	y_2	$w_2 \times y_2$	...	z_2	$w_2 \times z_2$	
.	.	.	.	.	.	.	.	
i	x_i	$w_i \times x_i$	y_i	$w_i \times y_i$	...	z_i	$w_i \times z_i$	
SUM	$\sum w_i \times x_i$		$\sum w_i \times y_i$		...	$\sum w_i \times z_i$		
SOLUTION:								
$\max\{\sum(w_i \times x_i), \sum(w_i \times y_i), \dots, \sum(w_i \times z_i)\}$								

Methods based on value analysis allows determination the storage site location, i.e. finding a set of alternative solutions based on relevant factors whereby alternative solutions can be ranked according to certain criteria, table 2. Ranking is possible when the defined values of some alternative solutions which are calculated on the basis of objective and subjective perceptions for each individual criterion. Given the fact that during the

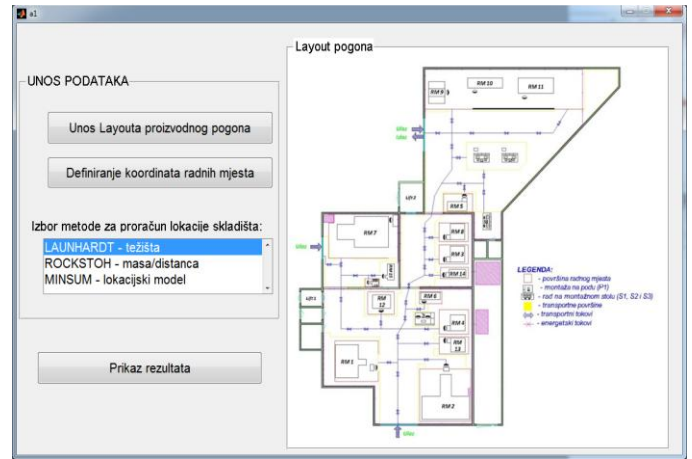
comparison of individual criteria is possible take into account simultaneously various factors and units, the value of the solution is therefore expressed dimensionless. This fact and the possibility of taking into account a large number of different criteria for selecting storage site locations is one of the basic advantages of applying these methods. There are numerous literary examples of usage of methods based on value analysis such as: [4] the steps of realization of the value analysis are specified, [6] the application of value analysis is presented in selecting the optimal storage site location at the design stage, [7] the criteria and the choice of factors to determine the storage site location are presented, etc.

The methods of selecting a storage site location on the basis of investment costs are based on the fact that the best storage site location in the production facility is the one that provides the largest profit for the invested capital. Based on the costs of production, income and production capital, the profitability of a certain storage site location is determined according to the form [8]:

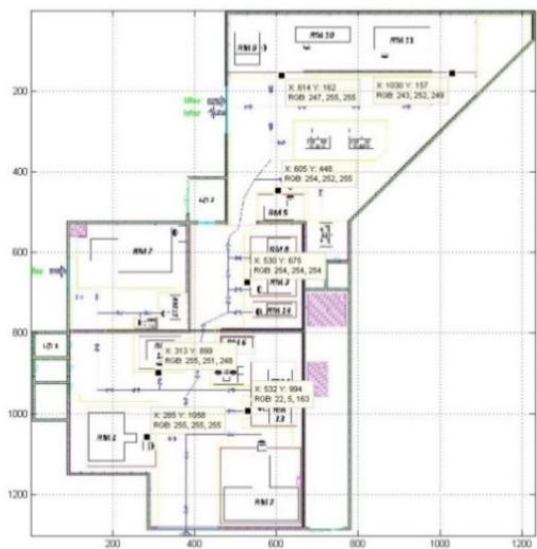
$$R_{VK} = \frac{U_p - C_{VK}}{V_K \cdot n_{VK}} \cdot 100$$

, where are:

R_{VK} – profitability of own capital, [%]
 U_p – total incomes, [nj]
 C_{VK} – total costs, [nj]
 V_K – the own capital, [nj]
 n_{VK} – the rate of own capital.



a)



b)

Fig. 2 a) GUI with production facility layout used to determining of the storage site location, b) Overview of the defined positions of the supplier/users of storage service within the observed production facility

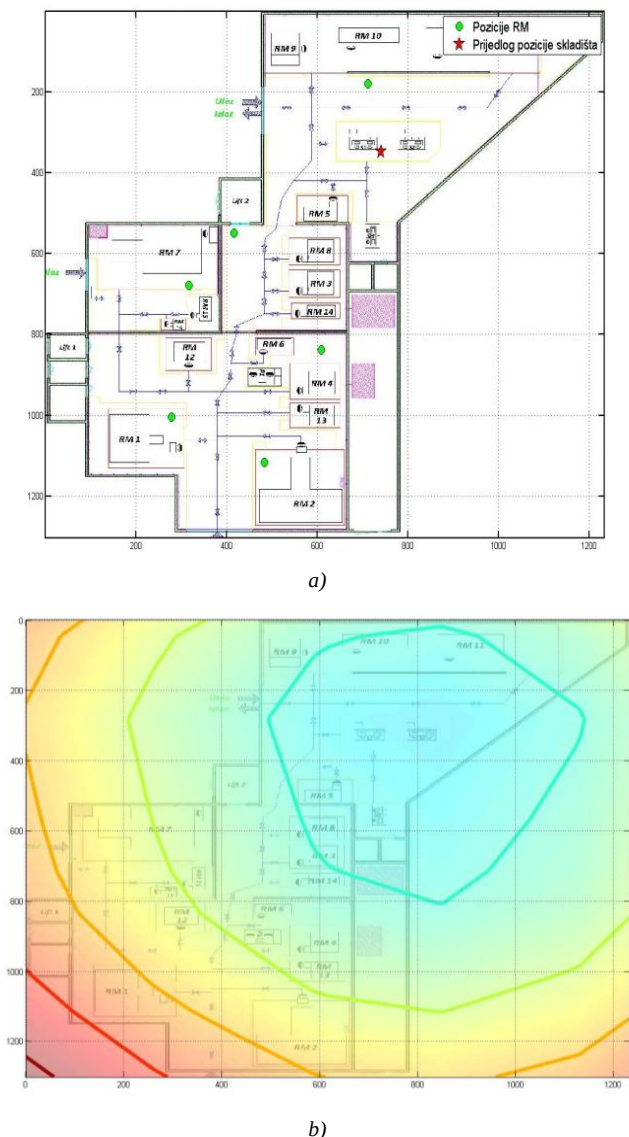
The application of this method also has certain deficiencies such as: the necessity of a long-term and extensive preparation of cost and revenue data that needs to be updated and detailed, additionally for determining of storage site location only the criteria that can be quantified are taken into account ,

while others criteria are neglected.

In addition to the aforementioned methods, other methods, such as multicriterial analysis, may be used to determine the storage site location with more or less success.

3. Practical example of determining of auxiliary storage site location by developed software solution

Depending on specific implementation conditions, afore presented methods, give some results that in the function of their specificity vary in a certain range. Regardless of this fact, all methods require a significant engagement in the collection, analysis and analytical processing of a number of parameters that may vary in a fairly wide spectrum. Commonly used approach in order to accelerate and improve such procedures is based on development of user software solutions. In this way, the user is relieved of the demands of mathematical processing of a large number of data, enabling him to be focus on qualitative aspects and multicriterial analysis of a particular problem. In accordance with the foregoing, a user application for the determining of storage site locations in the production facilities in the software package *Matlab* has been developed.



determined location of the storage site within the production facility. In a real production environment, the transportation routes within the production facilities are complex paths whose lengths are not uniquely determined by either the coordinate points or the Euclidean spacing, and that fact is necessary to take account during the interpretation of the presented solutions.

Notwithstanding the above, it is important to emphasize that the solution presented in this paper, despite some drawbacks and additional opportunities for its improvement, however represents a universal IT tool applicable to the solution of concrete problem of determining the storage site location in any layout of production facility presented and entered in an appropriate form -*.jpg format.

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pH AND TEMPERATURE INFLUENCE ON PHENOL REMOVAL FROM WATER BY HORSERADISH PEROXIDASE

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Abstract: Horseradish peroxidase represents one of the most exploited enzymes in the process of enzymatic phenol removal from aqueous solutions. It has a catalytic ability over a broad pH range, temperature and contaminant concentration. In this study we have investigated the influence of pH and temperature on process of phenol removal by crude horseradish peroxidase from aqueous solution. Reaction was performed in the presence of low molecular polyethylene glycol (PEG 300) at different temperatures (4, 12, 17, 20, 25, 30, 35, 40 and 45 °C) and pH values (3, 4, 5, 6, 7, 8 and 9). Reaction was monitored by measuring of absorbance changes of the samples taken at certain time intervals from reaction mixture. Obtained results shown that phenol removal from aqueous solution increases by temperature increase up to 35 °C, after which this effect no longer exists. Also, phenol removal increases in the pH range of 3 - 7, while a further increase of pH value leads to the opposite effect. Based on this it can be concluded that phenol removal from aqueous solutions greatly depends of peroxidase activity, because this temperature and pH values represents the optimum values of peroxidase enzymatic activity.

KEYWORDS: PHENOL REMOVAL, HORSERADISH PEROXIDASE, pH, TEMPERATURE

1. Introduction

Phenols belongs to a group of compounds that important for the environment because they possess a toxic and carcinogenic properties [1–3]. Due to their widespread applications, they are present as pollutant in many industrial wastewater streams [2,4,5]. Although there are many conventional methods for removal of phenolic compounds from wastewaters that include chemical, physical and biological processes, they are not always applicable [1,6]. From these reasons methods that includes enzyme for wastewater treatment were developed and enzymes such as peroxidases, laccases and polyphenol oxidases usually were used [2,7,8].

First application of horseradish peroxidase (HRP, EC 1.11.1.7) in the process of phenolic compounds removal from aqueous solutions, by Klibanov and collaborators (1980) was proposed [9]. Advantages of HRP on the other enzymes, it is a catalytic ability in wide range of pH and temperature as well as and contaminant concentrations [7,10]. In the presence of hydrogen peroxide HRP could catalyze the oxidation of different aromatic compounds such as phenols, biphenols, benzodioxines, anilines and related heteroaromatic compounds to form phenoxy radicals [11,12]. Created phenoxy radical products spontaneously polymerize to water-insoluble polymers that can be separated from solution by filtration or sedimentation [12–15].

Unfortunately, as other conventional methods for removal of phenolic compounds from wastewater, enzymatic process also have limitations [10]. One of the biggest problems is excessive treatment cost appears because the high cost of the purified enzyme and the potential formation of residual products in the aqueous phase [10]. This problem can be reduced using of protective additives and potentially inexpensive enzymes sources [10,12,16].

In addition to the previously mentioned problems, inactivation of HRP during the process of phenol removal also was a major problem. As Klibanov and Tu (1983) reported phenoxy radicals formed during the oxidation process, attack the catalytic active center of HRP which lead to the reduction and/or elimination of its catalytic ability [17]. The second hypothesis belongs to Nakamoto and Machida (1992) which assumed that inactivation of HRP was a consequence to a lack of contact between the substrate and enzyme, because HRP was captured in the newly formed polymer [18]. In some way, they managed to confirm their hypothesis because they showed that enzymes lifetime can be extended in the presence of highly hydrophilic additives with a higher affinity to the hydroxyl groups of the emerging polymer compared to HRP. Polyethylene glycol (PEG) and gelatin were particularly suitable because they could attack the polymer and thereby enable the enzyme to stay active in the solution. Results from investigations of Cooper and Nicell (1996) were demonstrated that crude extract from horseradish

roots and high purity enzyme have similar removal potential in reaction of total phenols removal [12]. Also, almost all cases the crude extract achieved better total phenols removals than the pure HRP for the same enzyme concentrations except at the point of maximum removal [12].

The aim of this paper was to investigate the influence of temperature and pH on peroxidase activity, extracted from horseradish (low purified), as well as on the process of phenol removal in the presence of hydrogen peroxide and low molecular polyethylene glycol (PEG 300) from aqueous solutions.

2. Materials and Methods

2.1. Enzyme isolation

2 g of horseradish root (*Armoracia rusticana* syn. *Cochlearia armoracia*, found in the local market) is cleaned and chopped, and extracted during the period of 30 min with 20 ml 100 mM phosphate buffer (pH 7.0) at room temperature (20 °C). After extraction, the centrifugation is performed 15 min at 3000 rpm. The obtained supernatant is transferred to a test tube and the rest of the plant material is subjected to extraction again. Stock enzyme solutions are stored at 4°C and warmed to room temperature immediately prior to use.

2.2. Experimental protocol

Phenol oxidation reactions were carried out in glass flasks at different temperatures (4, 12, 17, 20, 25, 30, 35, 40 and 45 °C) and pH values (3, 4, 5, 6, 7, 8 and 9) using 30 ml reaction volumes. Reaction mixtures contained 2.0 mM phenol, 300 mg/ml PEG and 1.2 U/ml sample of HRP. After 60 minutes, aliquots are pipetted into the tubes and HRP activity and phenol content were examined.

2.3. HRP activity assay

Peroxidase activity is determined by method of Soysal and Söylemez (2005), with slight modifications [19]. 2.1 ml of 100 mM acetate buffer (pH 7.0) is measured, followed by addition of 0.2 ml sample solution, 0.2 ml of 0.125% solution of *o*-dianisidine in methanol; the mixture is vigorously vortexed, and reaction is started by addition of 0.5 ml 8.8 mM H₂O₂. Absorbance change is recorded as a function of time at 460 nm, and activity of HRP is calculated by using following equation:

$$A[U/ml] = \text{tg}\alpha \cdot R/\varepsilon \quad (1)$$

where:

tg α - slope of the plot,

R - the total ratio volume of the reaction mixture and the enzyme volume,

ε - molar extinction coefficient ($\varepsilon_{460} = 11.3 \text{ mM}^{-1} \text{ cm}^{-1}$).

The blank contained all reagents except the hydrogen peroxide, which is replaced by aqua destillata.

One unit of peroxidase activity is defined as the amount of enzyme that transformed 1 μ mol of *o*-dianisidine per minute.

2.4. Phenolic compound assays

Phenol content is determined as described by Nicell et al., (1995), with slight modifications [13]. Aliquots (2.5 ml) from batch reactions are pipetted into the tubes at different time intervals (20, 40, 60, 80, 100 and 120 min) and reactions are stopped by adding 2.5 ml 96% ethanol solution. After, samples are treated with alum and pH is adjusted to 6.3 to optimize precipitation, using a stock solution of 0.1 M NaOH and 0.1 M HCl. Samples are centrifuged 10 min at 10000 rpm. Residual phenol concentration are determined by direct spectrophotometric measurement of the absorbance at 269 nm on UV-VIS.

3. Results and Discussion

In previous research of Savic and collaborators (2014) [20], phenol removal from aqueous solutions by raw peroxidase (extracted from horseradish) in the presence of hydrogen peroxide and PEG 300 as well as the influence of PEG 300, phenol and hydrogen peroxide on HRP activity and phenol removal was investigated. Obtained results were demonstrated that the presence of PEG 300 shows a stabilizing effect on HRP activity. The highest phenol removal was achieved when the concentrations of PEG 300, phenol and hydrogen peroxide were 300 mg/L, 2.0 mM and 2.5 mM, respectively, and that was the reason to select the same concentrations of the reaction participants for further research.

This study represent a continuation of previous research and in this study the influence of temperature and pH on peroxidase activity, as well as and their influence on the process of phenol removal in the presence of hydrogen peroxide and low molecular polyethylene glycol (PEG 300) from aqueous solutions were investigated.

Results from investigations of temperature influence on HRP activity on Fig. 1 were presented. Based on obtained results it could be concluded that there are three regions of HRP activity changes: first region from 4 to 20 °C with a intensive increasing of HRP activity, second from 20 to 35 °C with small changes of HRP activity, and third from 35 to 45 °C with decreasing of HRP activity. These results are in agreement result reported by Veitch (2004) where the highest activity was at 35 °C [21].

Obtained results from investigations of pH influence on HRP activity were presented on Fig. 2. Results indicate that increasing of HRP activity from 3 to 6 was progressive, between 6 and 7 changes were small, while at higher pH values HRP activity decreases. Also, if we take into account previously reported results of Veitch (2004) at different range of pH values, it can be concluded that results from our study are in agreement [21].

Influences of temperature and pH on phenol removal by HRP on figures 3 and 4 were presented, respectively. By looking of Figure 3 it can be noticed that the amount of phenol removed have two different parts. In first, with increasing of temperature (from 4 to 35°C) removed phenol amount also increases, even up to 66% from starting concentration, and second, where increasing of temperature leads to a reduction in the removed amount of phenol. If we take into consideration results from investigations of temperature influence on HRP activity, it could be concluded that changes of HRP activity with increasing of temperature were similar as achieved changes in the removed amount of phenol. A similar conclusion can be made by looking figures 2 and 4. Changes of HRP activity induced by changes of pH values follow changes in the removed amount of phenol. Based on these results, it can be concluded that phenol removal in great measure depends of HRP activity.

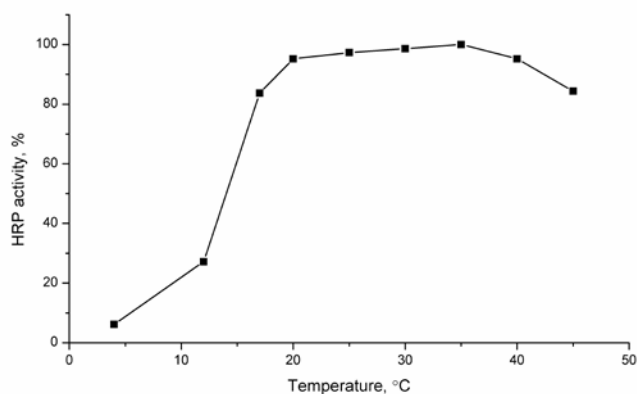


Fig. 1. Changes of HRP activity with temperature.

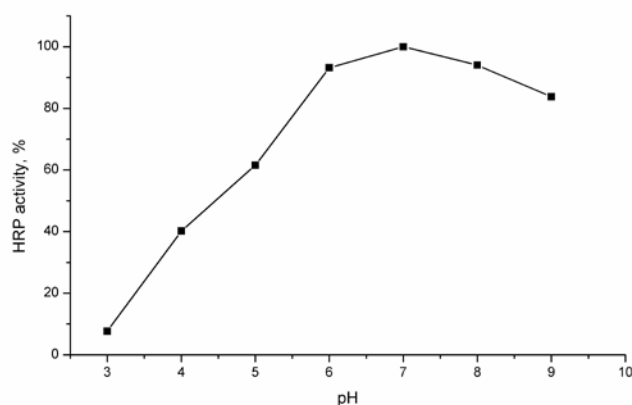


Fig. 2. Influence of pH on HRP activity.

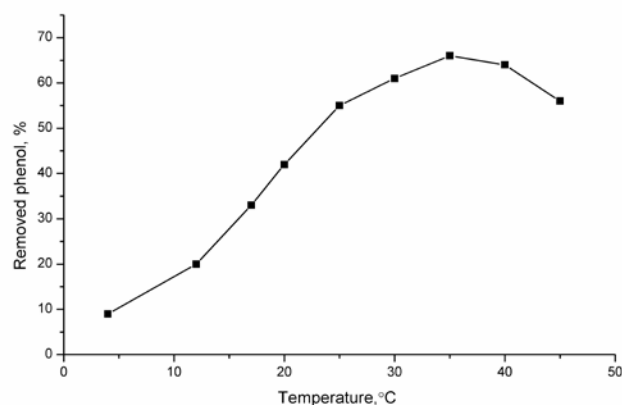


Fig. 3. Phenol removal by HRP at different temperatures.

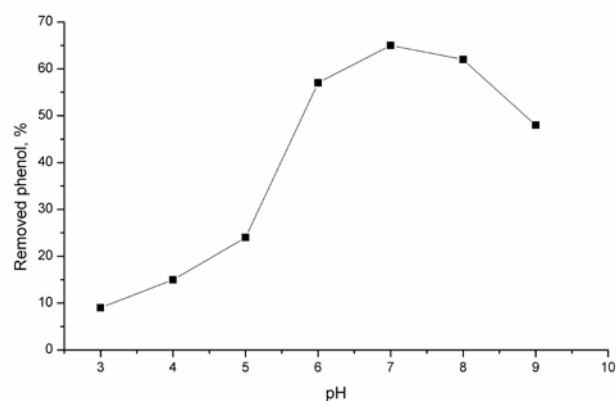


Fig. 4. Influence of pH on phenol removal by HRP.

4. Conclusion

Based on obtained results it could be concluded that phenol removal from aqueous solution increases by temperature increase up to 35 °C, after which this effect no longer exists. Also, phenol removal increases in the pH range of 3 - 7, while a further increase of pH value leads to the opposite effect. Based on this it can be concluded that phenol removal from aqueous solutions greatly depends of peroxidase activity, because this temperature and pH values represents the optimum values of peroxidase enzymatic activity.

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FULL USE OF MATHEMATICS – FOUNDRY

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Abstract: In this work, we present the necessity of using the full mathematics in the industrial branch of machine building of the example of the foundry. Obtaining the necessary structures is accompanied by research work even in micro-foundries, which is provided by powerful and new software products, i. knowledge transfer with computational mathematics, physics and education.

Keywords: MACHINE BUILDING, FOUNDRY, CASTING STRUCTURES, MATHEMATICS, EDUCATION

1. Introduction

The importance of mathematics is represented by a general block diagram of "The History of the Development of Knowledge of Civilization from Antiquity to Today" of Fig. 1

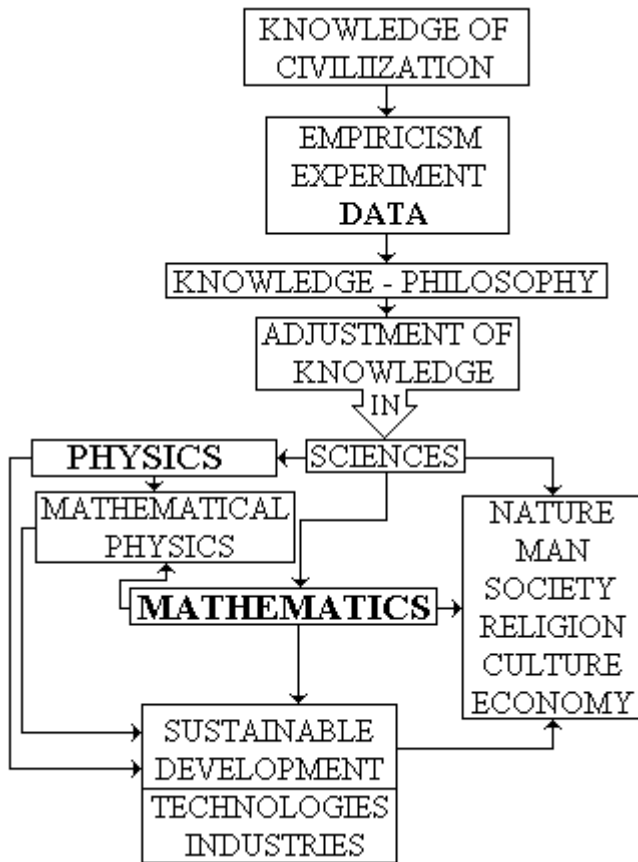


Fig. 1 Block diagram - Developing the knowledge of civilization from antiquity to today [1, 3, 4].

1 follows: 1. Initial knowledge is obtained through empiricism - obtaining and classifying experimental data; 2. Collecting knowledge in philosophy; 3. Knowledge is divided into separate sciences after Christ: 3.1 Physics - 18th Century; 3.2 Mathematics - the 19th and the beginnings of the 20th century; 3.3 Mathematics - Self Development; 3.4 Mathematics - a powerful tool for research: Description of physical processes and phenomena. Any theory is obtained only by using mathematics; 3.5 The term mathematical physics includes natural and theoretical physics; 4. Mathematics is in every area of human activity; 5. Sustainable development of civilization is based on: a sustainable society and economy - a challenge for every government; 6. Civilization only evolves by overcoming crises in society and the economy; 7. The challenge is the restructuring of the world by the fourth industrial revolution [1], involving education throughout every person's life, environmental technologies and industries.

The natural systems and the four main types of interaction forces in nature are classified in Fig. 2

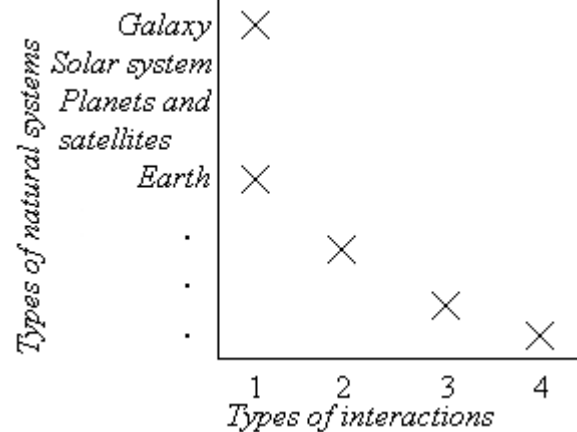


Fig. 2 Scheme - Natural systems and types of interactions [2]: 1 - gravitational interaction (large-scale events in the Universe), 2 - electromagnetic interaction (holds electrons in atoms and binds atoms to molecules and crystals (chemistry, biology)), 3 - strong interaction connects the nucleons (it unites protons and neutrons in the nucleus of all elements), 4 - weak interaction determines the forces acting between the light particles (leptons: electrons, neutrinos and muons) and between leptons and heavier particles).

The purpose of this work is to present the necessity of the complete mathematics in the foundry.

2. Foundry - physical and technological processes of structure formation

The casting structures are obtained in phase transition of 1st order is shown with the characteristic scale of the scheme of Fig. 3

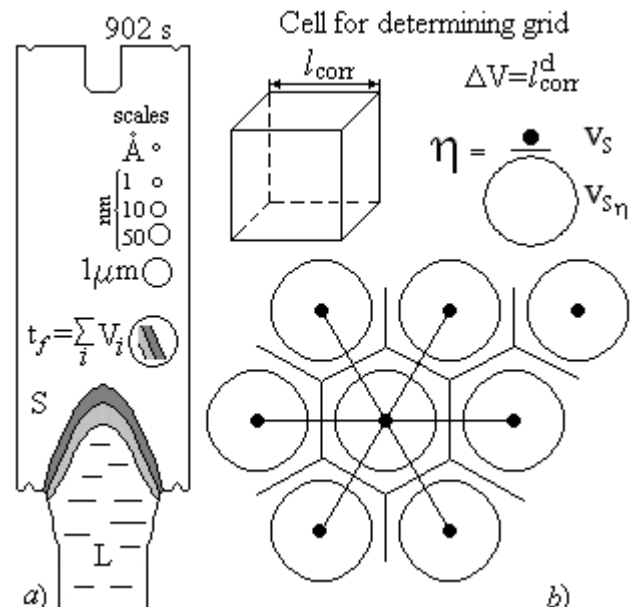


Fig. 3 The casting structures are obtained in phase transition of 1st

order (solidification) [5]: a) Numerical experiment: technological solidification of a cylindrical cast at 902 s, graphically represented by the geometry of the solidification zone (front) – ΔV_i between the liquid (L) and the solid (S) phases. Scales $\text{\AA}$, nm, $1\text{ }\mu\text{m}$. t_f – local time of solidification. V_i – chosen local volume for description of structure formation; b) Cell for determining grid – l_{corr} for V_i , ΔV_i – changing the volume V_i from melting (solidification), d – direction of growth 1D, 2D or 3D, η – packing density coefficient, v_s – volume of atom, $v_{s\eta}$ – volume cell, Wigner-Zeit cell and structure.

The technological system of foundry we introduced on the example by the machine – Gas counter-pressure casting method Fig. 4

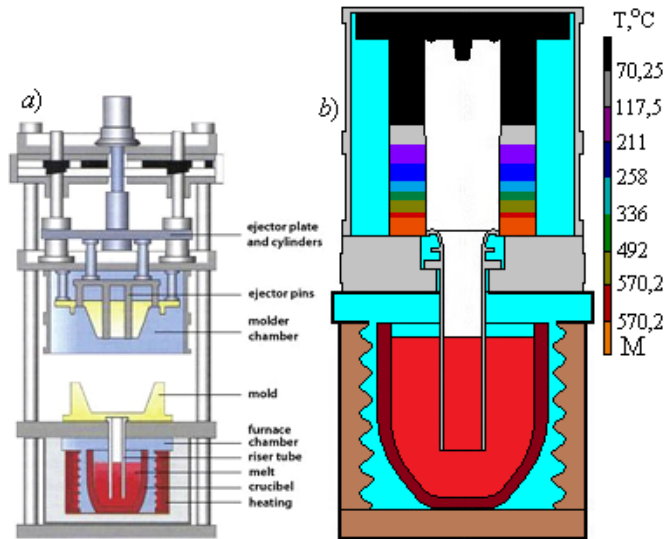


Fig. 4 Casting technology system - Gas counter-pressure casting machine: a) General appearance of the casting machine; b) Technology for producing counter-pressure cylindrical castings. The technological regime shown (see Fig.2 a) is obtain with initial temperature of the mould without taking into account the filling process.

The technological system (see Fig. 4) provides of macro-level to obtain the desired structure *average diameter of polycrystalline grains* [12]. Макропараметрите на лярската технология са преохлаждането на стопилката и скоростта на разсейване на скритата топлина на топене [5]. The macro-parameters of the casting technology are **the overcooling of the melt** and **scattering of the latent heat of melting** [3, 5, 11, 12].

3. Mathematics in Foundry

A scale of $1\text{ }\mu\text{m}$ is a macro-scale. Scale for nm or $\text{\AA}$ requires modern methodologies based on [8, 9, 10]. Обобщено това е математиката, теоретичете и математичната физика представено на Фиг.

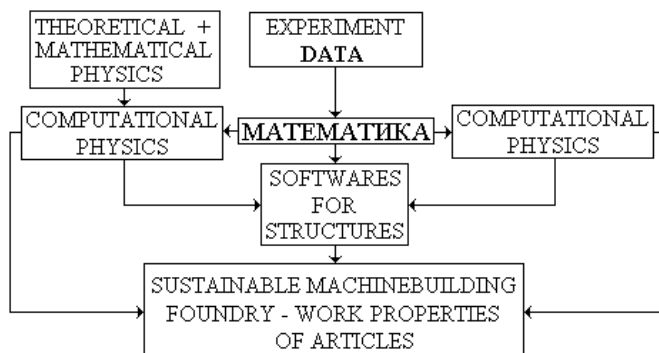


Fig. 5 Scheme - Full mathematics is needed in Micro-Foundry and Industry 4.0.

Full mathematics is called upon to create new purely mathematical theories. The new theories are evolving because Gödel's theorems of "incompleteness" clearly show that there is no complete mathematical theory. The history of mathematics shows the need for the development of pure mathematics, but it is challenging to suggest the assessment of the development of the necessary, for example, a "new mathematical field".

4. Conclusion

Mathematics is a powerful tool for research. Mathematics is needed in public development, for example "virtual factories", apart from technological, legal relations between companies, based on new experimental data, evaluations are also made for research ideas for development from "artificial intelligence". Hence Industry Change 4.0: "factories without people", and people naturally need life-long education.

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THE METHODOLOGY FOR VEHICLES PARKING ANALYSIS: CASE STUDY – CITY OF PRISHTINA

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Abstract: Cities are faced with many challenges, in particular in relation to the mobility of people and the structure of land-use. Parking management, which makes the link between the fields of urban planning and transportation, is one of the crucial ways to meet these challenges.

The problem of parking in the capital of Kosovo in Prishtina is a major concern for the citizens and central and local authorities. For the purpose of easier parking problem study, the first ring of the center zone of Prishtina is divided into XI sub zones. During the collection of data directly from XI sub zones through the observation- survey method, it was noted that the biggest problems are in the sub zones II. Therefore, in this paper is analyzed sub zone II through the parking statistics such as parking causes, accumulation, parking loads, parking duration. After the analysis, findings are made on the choice of the parking problem for this sub zones.

Keywords: DESIGN, SUSPENSION SYSTEM, OPTIMIZATION, MODELING, CAD

1. Introduction

The paradox of transportation vehicles is that they are most studied when they are the least used, i.e. when they are in motion, while they spend most of their time stationary or parked. For example, taking into account only the commute to work, which was measured to be on average 27 minutes by car in the six largest Canadian census metropolitan areas [1]. There are several reasons to despite the importance of the phenomenon, “parking is the unstudied link between transportation and land use”, an essential one being the cost or difficulty to collect or have access to such data.

Data collection in the field of parking studies is a major challenge. The diversity of parking types and the multiple variations of their vocations contribute to this difficulty. In the literature there are several methods of data collection to analyze the parking spaces: Roess, Prasas and McShane provide a standard textbook approach to parking data collection and analysis [2]. Putnik has a text book for methods of Data collection and analysis [3]. Authors Morency et al. [4] and Tong et al. [5] have proposed a methodology to estimate parking capacity in various areas using travel survey data. Their method relies on the spatial-temporal monitoring of cars in the region using declared car driver trips. With their 5 % sampling, the Montreal travel surveys have sufficient data to allow for specific analysis. The method also relies on declared information on the type of parking space used at the destination. It is hence possible to cumulate cars in space throughout a typical day and to estimate a theoretical parking capacity using the maximum number of cars simultaneously parked in an area.

After the last war (1998-1999), the Republic of Kosovo has undergone major socio-political changes marked by economic and demographics, but also by profound social and cultural transformation, changing lifestyles and forms of movement in Kosova cities. One of the most significant changes in the urban area is the urban mobility. Increase the number of private cars is a lasting trend in Kosova city, this reflects the increased standard of living and growing demands for free choice of lifestyle and movement.

Urban mobility includes the mobility of people and goods in the road infrastructure of the city, and placement process, waiting and parking. Prishtina as the administrative, university and economic capital of Kosovo besides its internal urban load, during all time periods and at an uninterrupted interval of 24 hours, is populated by citizens from all sides, whether with a daily stay or longer stay. Current road infrastructure despite the maximum modifications to the rational use of parking spaces, does not allow for large parking spaces.

The data required for parking problem analysis are taken directly from XI sub zones under the first ring of the center zone of

Prishtina through the observation- survey method on certain days in the time period from 6:00 to 18:00 [6].

This paper has been analyzed sub zone II through the parking statistics such as: accumulation, parking loads, parking time, parking turnover, and the cause of parking.

2. Methodology of analysis

In order to better analyze the problem of parking, the first ring of the centers zone of Prishtina is divided into XI sub-zones (Figure 1). The first ring has a circumference length of about 4650 m and is bordered by the streets:

- The “KLA” Street with a length of 800 [m],
- “Agim Ramadani” Street with length 150 [m],
- The Street "Boulevard Bill Clinton" with a length of 950 [m] and
- "Tirana" Street with a length of 1400 [m].



Figure 1. First ring of the center zone of Prishtina [6]

The purpose of the study was to analyze the parking statistics of some parking areas (subzone II) and current state of affairs, primarily serving the administration, education and business, where during the day a large number of incoming cars within the working day is gathered. Also examine a large number cowering with residential where an introduction of paid parking is planned.

Inventory of parking places is done by walking around the site and affixing them to the card, observing and reporting the parking position. A complete inventory of parking capacity for the subzones II (Figure 2) was made, and we got a real and current picture of the situation with absolute capacity of parking places required in the venue areas. Census of all parking cars, it is very important to define the capacity for future and implementation of parking policy.

Drawing and numbering of all locations for parking is particularly important, because we need to consider all parked cars and to indicate the category of parking place. Four parking places (Figure 2 - E, A, M and PG) have been identified.

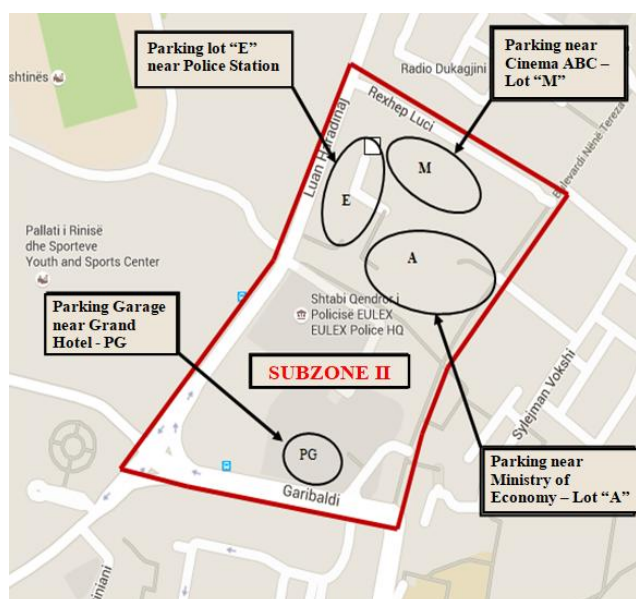


Figure 2. Sub zone II of the first ring of the Center Zone in Prishtina with parking places (Lots) E, A, M and PG [6].

To collect the parking data for statistic purposes, are used these methods:

- In-out survey,
- Fixed period sampling,
- License plate method of survey.

In this work is used *In-out survey method*. This method helps to find:

- Occupancy count in the selected parking lot is taken at the beginning,
- Number of vehicles that enter the parking lot for a particular time interval is counted,
- Number of vehicles that leave the parking lot is also taken
- Final occupancy in the parking lot is also taken,
- Data regarding the time duration for which a particular vehicle used that parking lot is obtained,
- Parking duration and turnover is obtained.

Observing the location for sub-zones II is done date 01.06.2014 for parking lots E, A, dhe M and date 12/31/2016 for parking lots "PG", started at 6:00 pm at 18:00 [6].

3. Results and analysis of parking statistics

In order to solve the problem of parking firstly, it is necessary to study and plan the parking statistics that are closely related to the parking and based on the data obtained we can approach the solution of the parking problem.

Parking statistics are: accumulation, parking loads, parking duration, parking turnover, reason of parking. For parking lots E, A, M and PG statistics are analyzed particularly for each.

Accumulation can be found out as initial count plus number of vehicles that entered the parking lot till that time minus the number of vehicles that just exited for that particular time interval.

Parking load obtained by simply multiplying the number of vehicles occupying the parking area at each time interval with the time interval

Average parking duration is Ratio of total vehicle hours to the number of vehicles parked.

Parking index also called occupancy or efficiency is Ratio of number of bays occupied in time duration to the total space available. An aggregate measure of how effectively the parking space is utilized.

Parking turnover is ratio of number of vehicles parked in duration to number of parking bays available.

3.1. Parking lot E

Results gained from survey in the location for parking lot "E" is shown in tabular form (Table 1). In tables 1 is calculated accumulation and occupancy.

Time	Entry	Exit	Accumulation	Occupancy
06:00-07:00	0	0	50	83.30
07:00-08:00	5	4	51	85.0
08:00-09:00	11	6	56	93.30
09:00-10:00	15	10	61	101.60
10:00-11:00	26	20	67	111.70
11:00-12:00	18	15	70	116.60
12:00-13:00	0	0	70	116.60
13:00-14:00	52	16	106	176.60
14:00-15:00	27	36	97	161.60
15:00-16:00	16	22	91	151.50
16:00-17:00	19	17	93	155.00
17:00-18:00	5	11	87	145.00
Total	194	157	244	124.80

Table 1. Accumulation and occupancy in the parking lot "E"

Based on Table.1, it can be concluded that at the start of survey were parked exactly 50 vehicles. During the day time in this parking have entered 194 vehicles, and exited 157 vehicles. Accumulated vehicles that have occupied this parking lot during the day is 244 vehicles.

In Figure 3 is shown accumulation of the parking lot E, with legal number of bays 60.

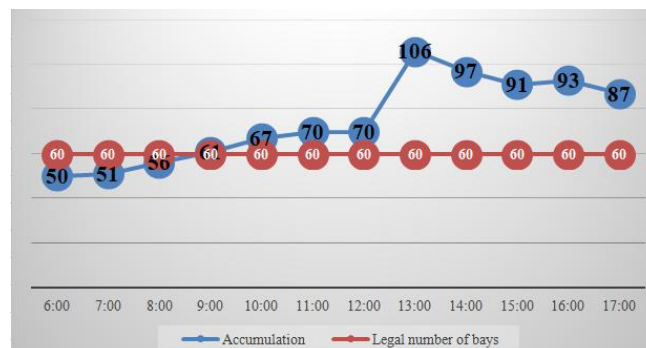


Figure 3 Accumulation and legal number of bays at parking lot 'E'

Based on Figure 3, can be concluded that higher number of vehicles in the parking is in time interval between 13:00 to 14:00, with total of 106 vehicles. Demand for 106 parking places needs to be regulated through parking policies and solving the problem of resident inhabitants.



Figure .4. Actual parking situation of vehicles in the parking lot 'E'

In the Figure. 4 is shown actual situation in the parking Lot “E”, and it corresponds to calculations shown above.

Results of the survey in the location, at the parking lot “E”, about parking duration are shown in table 2. Results gained for parking load and relative dispersion in % of parking duration are shown in the same table.

<u>Parking duration (h)</u>	<u>Number of vehicles</u>	<u>Relative dispersion %</u>	<u>Parking load</u>
Up to 1h	57	25.79	57
1 h up to 2 h	33	14.93	66
2 h up to 3 h	12	5.42	36
3 h up to 4 h	15	6.78	60
4 h up to 5 h	21	9.50	105
5 h up to 6 h	7	3.16	42
6 h up to 7 h	9	4.07	63
7 h up to 8 h	9	4.07	63
8 h up to 9 h	8	3.61	72
9 h up to 10 h	4	1.80	40
10 h up to 11 h	4	1.80	40
11 h up to 12 h	21	9.50	252
More than 12 h (Calculations for 12 h)	21	9.50	252

Table 2. Parking duration of vehicles per hour (h), in the Parking Lot “E”

Higher percentage of 25.79% have parking duration up to 1h. Selection of parking duration up to 2 hours includes 40.72% of parked vehicles.

Reason of parking is close to the destination, parking without fee, residence (living flats), work (close to institutions), large number of coffee places, recreation, business, shopping, private matters, etc.

Time	Entrance	Exit	Accumulation	Occupancy
06:00-07:00	1	0	86	122,8
07:00-08:00	6	3	89	127,1
08:00-09:00	11	34	66	94,3
09:00-10:00	30	24	72	102,8
10:00-11:00	23	23	72	102,8
11:00-12:00	10	16	66	94,3
12:00-13:00	1	3	64	85,7
13:00-14:00	78	30	112	160
14:00-15:00	25	20	117	167,2
15:00-16:00	17	18	116	165,7
16:00-17:00	38	19	135	192,8
17:00-18:00	10	9	126	180
Total	250	199	336	143,6

Table. 3 Accumulation and occupancy in the parking lot “A”

Parking lot A

Results gained from survey in the location for parking lot »A« is shown in tabular form (Table 3). In tables 3 is calculated accumulation and occupancy.

Based on Table.3, it can be concluded that at the start of survey were parked exactly 85 vehicles. During the day time in this parking have entered 250 vehicles, and exited 199 vehicles. Accumulated vehicles that have occupied this parking lot during the day is 336 vehicles.

In Figure. 5 is shown accumulation of the parking lot A, with legal number of bays 70.

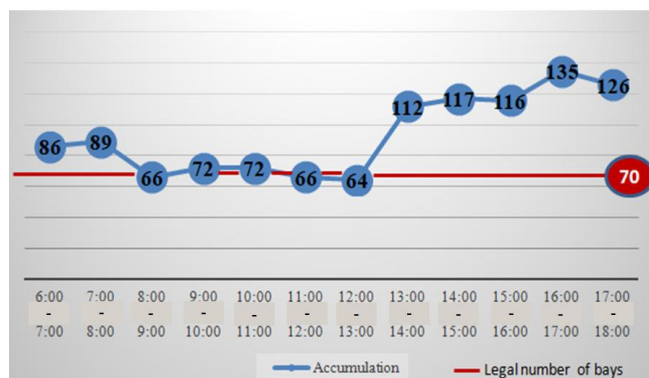


Figure 5. Accumulation and legal number of bays in parking lot ‘A’

Based on Figure 5, can be concluded that higher number of vehicles in the parking is in time interval between 16:00 to 17:00, with total of 135 vehicles. Demand for 135 parking places needs to be regulated through parking policies and solving the problem of resident inhabitants.



Figure 6. Actual parking situation of vehicles in the parking lot A

In the Figure. 6 is shown actual situation in the parking Lot A, and it corresponds to calculations shown above.

Results of the survey in the location, at the parking lot »A«, about parking duration are shown in table 4. Results gained for parking load and relative dispersion in % of parking duration are shown in the same table.

<u>Parking duration (h)</u>	<u>Number of vehicles</u>	<u>Relative dispersion in %</u>	<u>Parking load</u>
Up to 1h	108	40.75	108
1 h up to 2 h	23	8.67	46
2 h up to 3 h	20	7.54	60
3 h up to 4 h	23	8.67	92
4 h up to 5 h	33	12.45	165
5 h up to 6 h	12	4.53	72
6 h up to 7 h	14	5.29	98
7 h up to 8 h	10	3.77	80
8 h up to 9 h	5	1.88	45
9 h up to 10 h	4	1.55	40
10 h up to 11 h	1	0.38	11
11 h up to 12 h	6	2.26	72
More than 12 h (Calculations for 12 h)	6	2.26	72

Table 4. Parking duration of vehicles per hour (h), in the Parking Lot “A”

Higher percentage of 40.75 % have parking duration up to 1h. Selection of parking duration up to 2 hours includes 49.42 % of parked vehicles.

Reason of parking is close to the destination, parking without fee, residence (living flats), work (close to institutions), large number of coffee places, recreation, business, shopping, private matters, etc.

Parking lot M

Results gained from survey in the location for parking lot "M" is shown in tabular form (Table 5). In tables 5 is calculated accumulation and occupancy.

Time	Entry	Exit	Accumulation	Occupancy
06:00-07:00	0	0	31	73.8
07:00-08:00	9	0	40	95.2
08:00-09:00	15	10	45	107.1
09:00-10:00	14	18	41	97.6
10:00-11:00	24	7	58	139.2
11:00-12:00	7	16	58	139.2
12:00-13:00	2	6	54	128.5
13:00-14:00	33	25	58	139.2
14:00-15:00	24	24	58	139.2
15:00-16:00	15	19	54	128.5
16:00-17:00	14	16	52	123.8
17:00-18:00	16	32	36	85.8
Total	173	173	204	116.4

Table 5. Accumulation and occupancy in the parking lot "M"

Based on Table.5, it can be concluded that at the start of survey were parked exactly 31 vehicles. During the day time in this parking have entered 173 vehicles, and exited 173 vehicles. Accumulated vehicles that have occupied this parking lot during the day is 204 vehicles.

In Figure. 7 is shown accumulation of the parking lot A, with legal number of bays 42.

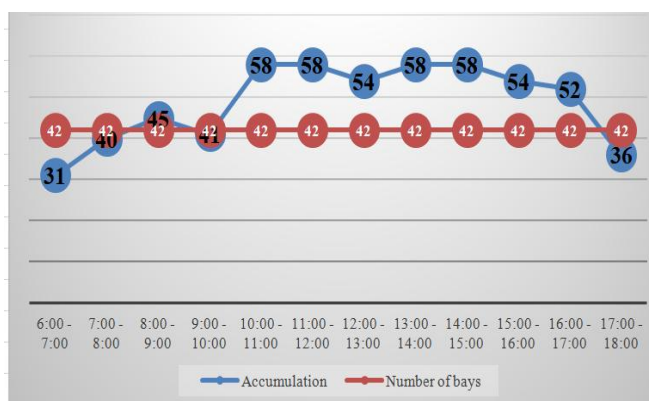


Figure 7. Accumulation and legal number of bays in parking lot M

Based on Figure 7, can be concluded that higher number of vehicles in the parking are in time interval between 10:00 to 12:00 and interval between 13:00 to 15:00, with total of 58 vehicles. Demand for 58 parking places needs to be regulated through parking policies and solving the problem of resident inhabitants.



Figure 8. Actual parking situation of vehicles in the parking lot "M"

In the Figure 8 is shown actual situation in the parking lot M, and it corresponds to calculations shown above.

Results of the survey in the location, at the parking lot »M«, about parking duration are shown in table 6. Results gained for parking load and relative dispersion in % of parking duration are shown in the same table.

Parking duration (h)	Number of vehicles	Relative dispersion in %	Parking load
Up to 1h	100	47.39	100
1 h up to 2 h	47	22.28	94
2 h up to 3 h	17	8.1	51
3 h up to 4 h	11	5.21	44
4 h up to 5 h	8	3.79	40
5 h up to 6 h	2	0.94	12
6 h up to 7 h	0	0	0
7 h up to 8 h	2	0.94	16
8 h up to 9 h	3	1.42	27
9 h up to 10 h	2	0.94	20
10 h up to 11 h	5	2.36	55
11 h up to 12 h	1	0.47	55
More than 12 h (Calculations for 12 h)	13	6.16	156

Table 6. Parking duration of vehicles per hour (h), in the Parking Lot "M"

Higher percentage of 47.39 % have parking duration up to 1h. Selection of parking duration up to 2 hours includes 69.67 % of parked vehicles.

Reason of parking is same with parking lots E and A, close to the destination, parking without fee, residence (living flats), large number of coffee places, recreation, business, shopping, private matters, etc.

Parking garage PG

Results gained from survey in the location for parking garage »PG« is shown in tabular form (Table 7). In tables 5 is calculated accumulation and occupancy.

Time	Entrance	Exit	Accumulation	Occupancy
06:00-07:00	0	0	14	17,5
07:00-08:00	1	1	14	17,5
08:00-09:00	11	4	21	26,25
09:00-10:00	7	1	27	33,75
10:00-11:00	9	5	31	38,75
11:00-12:00	39	9	61	76,25
12:00-13:00	29	24	66	82,5
13:00-14:00	48	37	77	96,25
14:00-15:00	35	45	67	83,75
15:00-16:00	25	38	54	67,5
16:00-17:00	19	21	52	65
17:00-18:00	4	13	24	30
Total	227	198	241	52,91

Table 7. Accumulation and occupancy in the parking lot "PG"

Based on Table 7, it can be concluded that at the start of survey were parked exactly 14 vehicles. During the day time in this parking have entered 227 vehicles, and exited 198 vehicles. Accumulated vehicles that have occupied this parking lot during the day is 241 vehicles.

In Figure 7 is shown accumulation of the parking garage PG, with legal number of bays 80.

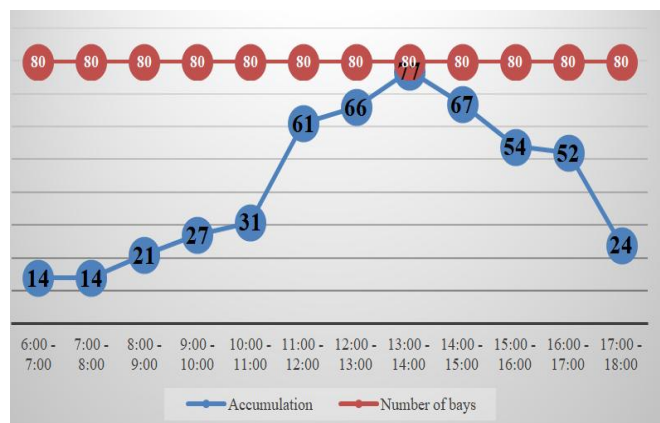


Figure 9. Accumulation and legal number of bays in parking lot PG

The reason for low average occupancy at 53 % is that parking is paid.

Based on Figure 9, can be concluded that higher number of vehicles in the parking are in time interval between 13:00 to 14:00, with total of 78 vehicles. Demand for parking places is not need.

Results of the survey in the location, at the parking garage "PG", about parking duration are shown in table 8. Results gained for parking load and relative dispersion in % of parking duration are shown in the same table.

Parking duration (h)	Number of vehicles	Relative dispersion in %	Parking load
Up to 1h	87	35.08	87
1 h up to 2 h	74	29.84	148
2 h up to 3 h	40	16.13	120
3 h up to 4 h	16	6.45	64
4 h up to 5 h	7	2.82	35
5 h up to 6 h	3	1.21	18
6 h up to 7 h	1	0.40	7
7 h up to 8 h	1	0.40	8
8 h up to 9 h	1	0.40	9
9 h up to 10 h	2	0.81	20
10 h up to 11 h	0	0.00	0
11 h up to 12 h	8	3.23	96
More than 12 h (Calculations for 12 h)	8	3.23	96

Table 8. Parking duration of vehicles per hour (h), in the Parking garage "PG"

Higher percentage of 35.08 % have parking duration up to 1h. Selection of parking duration up to 2 hours includes 64.92 % of parked vehicles.

Reason of parking is close to the destination, large number of coffee places, recreation, business, shopping, private matters, etc.

In Table 9 are shown results of parking statistics for parking lots E", "A", "M" and parking garage PG.

Parking statistics	Parking lot E	Parking lot A	Parking lot M	Parking garage PG
Average occupancy, %	124,8	143,6	116,4	53
Total parking load, h	4.7	2.86	3.28	2.93
Average parking duration, h	1148	962	670	706
Average parking turnover, -	4	5,6	5	3

Table 9. Parking statistics for parking lots "E", "A", "M" and parking garage PG

4. Conclusions

After results shown and analysed, conclusions are as follows:

- Average occupancy for parking lots "E", "A", "M" are more than 100 % respectively 124,8%; 143,6%; 116,4%, and for parking garage - PG is 53 %.

- Average parking duration for parking lots "E", "A", "M" are respectively 4,7 h; 2,86 h; 3,28 h, and for parking garage - PG is 2,93 %.

- Average parking turnover for parking lots "E", "A", "M" are respectively 4; 5,6; 5, and for parking garage - PG is 3.

Difference of parking statistics between parking lots "E", "A", "M" and "PG", is based on the fact that parking lots "E", "A", "M" are without payment fees, while parking garage is with payment fee.

In order to solve problem of parking lots E", "A", "M" it is recommended to build one additional parking garage for resident inhabitants, and to apply fees for parking bays in duration of 2 hours.

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MODELING OF SOLIDIFICATION IN RESISTANCE SPOT WELDING

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Abstract: In the present study a comprehensive numerical study has been conducted to simulate the resistance spot welding process. The phase- field method is employed to model the phase change during the melting and solidification of the material. By this way, the martensitic properties are assigned at the nugget and heat affected zone. As a result of this modelling the residual stress at the heat affected zone is attained and shows maximum value on the heat affected zone.

Keywords: RESISTANCE SPOT WELDING, RESIDUAL STRESS, NUGGET

1. Introduction

Resistance spot welding is a common technique to join the sheet metals in automotive industry [1]. Since the welding method is a thermal process, estimation of the residual stresses and consequently the fatigue of the joint need to analyze the phase change during the melting and solidification of the sheet parts. Available data in the literature reveals that a hard martensitic microstructure in nugget and heat affected zone around the nugget appear after the solidification of the joint [2,3]. In the present study, a comprehensive numerical model including the phase change is introduced to capture these transformations during the welding.

2. Numerical Model

In the resistance spot welding process, the electrical filed passes through the two electrodes which hold two metal sheets together by applying a mechanical force. The resulted resistance from the applied electrical field generates heat to increase temperature in the electrodes and sheets. Some pieces of the metal sheets are melted and joined together. During the cooling of the pieces the molten metal is solidified. But the specifications of the metal at the nugget (solidified metal) is different from the row material. It affects the mechanical properties of the welding parts such as the distribution of the residual stresses.

The governing equations for electrical, thermal and mechanical fields in cylindrical coordinate are

$$\begin{cases} \nabla \cdot J = Q_{jw} \\ J = \sigma E + J_s \\ E = -\nabla V \end{cases} \quad (1)$$

$$\begin{cases} \rho C_p \frac{\partial T}{\partial t} + \rho C_p u \cdot \nabla T + \nabla \cdot q = Q + Q_q \\ q = -k \nabla T \end{cases} \quad (2)$$

$$\begin{cases} \nabla \cdot FS + Fv = 0 \\ F = I + \nabla u \end{cases} \quad (3)$$

Boundary conditions are depicts in Table 1.

Welding Time	80 ms
Holding Time	480 ms
Electrode Force	4000 N
Applied Current	7 kA
Material of Sheets	AISI 316L
Materila of Electrodes	Cu-Cr Alloy

The phase-field method is used to model the two- phase (liquid and solid) and capturing the interface. During the solidification the mechanical properties of the material are replaced by martensitic properties. Figs. 1,2 illustrate the phase transition and von Mises stress distribution at the end of the welding time, respectively.

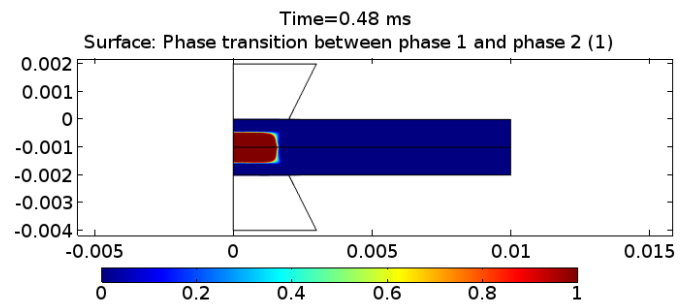


Fig. 1 Phase transition between solid (base metal) and liquid (molten metal)

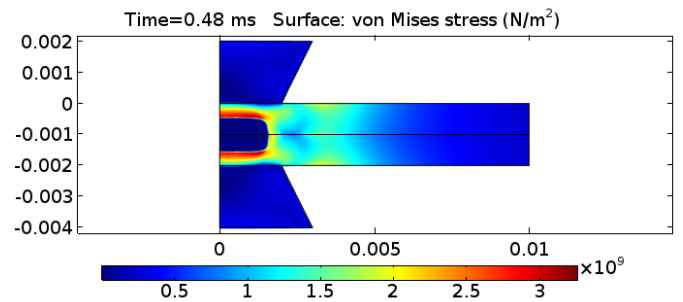


Fig. 2 Distribution of von mises stress at the end of welding time

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EFFECT OF ANNEALING TEMPERATURE ON MICROSTRUCTURE OF Ti-Al-V-Mo-Zr SYSTEM ALLOYS

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Abstract: Quantitative analysis of the phase composition of the Ti-Al-V-Mo-Zr system alloys was carried out during operation using the Thermo-Calc program (TCW5 version, TTTI3 database). Polythermal and isothermal cuts are plotted, design temperature values of liquidus, solidus and transition into β -field during heating are given. Regarding the titanium alloy of the Ti-Al-V-Mo-Zr system the effect of annealing temperature on the microstructure of the alloy as well as on the alloying elements content in α and β -phases was studied using the scanning electron microscopy method.

KEY WORDS: TI-AL-V-MO-ZR SYSTEM, TITANIUM ALLOYS, PHASE COMPOSITION, HEAT TREATMENT, MICROSTRUCTURE, ANNEALING

1. Introduction

Titanium alloys have a number of advantages compared to other alloys: availability of both high strength and ductility, low density ensuring high specific strength; heat resistance of up to 600 °C, high resistance to corrosion in aggressive environments [1, 3]. The required property package can be attained as a result of alloying of titanium alloys. The alloying elements contained in industrial titanium alloys together with titanium form substitutional solid solutions and change the temperature of allotropic transformation. The alloying of titanium allows increasing its strength by 2 or 3 times and sometimes increasing resistance to corrosion as well.

Polymorphism of titanium creates the opportunity to improve the properties of titanium alloys using heat treatment which allows enhancing their strength considerably with relatively small decrease of their ductility. The distinction of titanium alloys is that unlike steels annealing is the main type of heat treatment and the required strength is achieved during the formation of heterophase structures [3- 4].

In order to provide the required level of structural condition and properties of the titanium alloys being developed, it is necessary to carry out comprehensive theoretical and experimental research on scientifically based choice of their tailored compositions, advanced casting and treatment techniques. The purpose of the work was to study the Ti-Al-V-Mo-Zr phase diagram and the effect of heat treatment on the phase composition and structure of titanium alloys using both design and experimental methods. This research aims at the creation of a scientific base necessary for the validation of the composition of multi-component titanium alloys.

2. Preconditions and means for resolving the problem

2.1 Quantitative analysis of phase composition of Ti-Al-V-Mo-Zr system alloys

Polythermal and isothermal cuts are used for semi-quantitative assessment of the phase composition of multi-component alloys. For titanium alloys the analysis was carried out using the graphical technique [5]. However the possibilities provided by the graphical technique are rather limited, especially in the case of quaternary and more complicated systems. In this work polythermal and isothermal cuts of phase diagrams based on titanium were plotted with Thermo-Calc. Polythermal cuts

provide the opportunity to assess the effect of individual alloying elements on the lines of solidus and liquidus and the formation of the phase composition of the alloy during cooling and heating.

The calculation of polythermal cuts was made using constant concentration of vanadium, zirconium (1,3% V and 2 % Zr) and variable concentration of aluminium, molybdenum, which allows to determine the extent to which these alloying elements affect the temperatures of phase transitions, particularly the transition into the β -field during heating ($T_{\beta\beta}$). The fragments of polythermal cuts of the phase diagram of the Ti-Al-V-Mo-Zr system are shown in Figure 1.

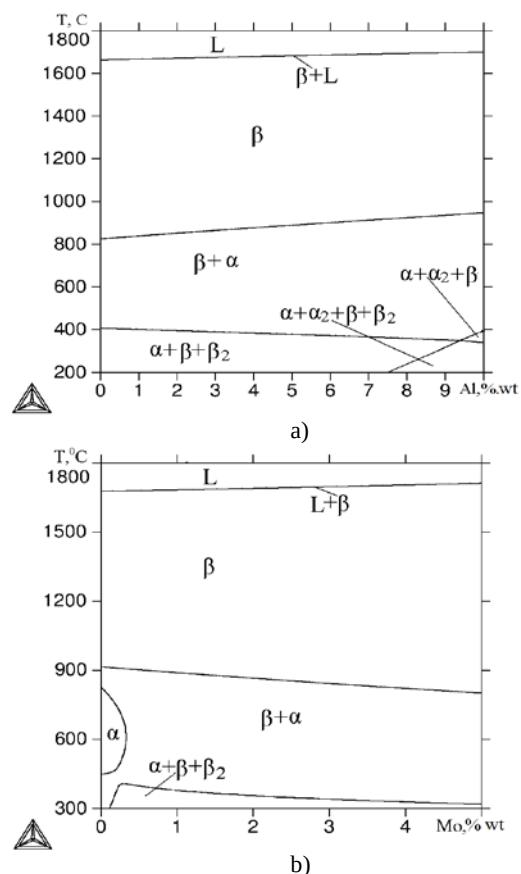


Figure 1 – Fragments of polythermal cuts of Ti-Al-V-Mo-Zr system phase diagram

a – 1.3 % V, 2 % Zr, 1.3 Mo; *b* – 6.5 % Al, 1.3 %V, 2 % Zr

Simulation demonstrated that when temperature is decreased a series of intermetallic phases is formed in the alloys being studied, in which case the alloys pass from a single-phase β – field via a two-phase $\beta + \alpha$ field into a three-phase $\alpha + \beta + \beta_2$ field and even a four-phase $\alpha + \alpha_2 + \beta + \beta_2$ field.

The significant characteristics of all alloys are the lines of solidus and liquidus that determine the melting, casting and heat treatment conditions. As indicated in the figure the interval does not exceed 5-6 °C in the Al and Mo concentration field being studied.

Imperfect crystallization, especially of titanium alloys, generally results in considerable deviation of individual sections of casting from the average value. Thus, castings are subjected to annealing; during the annealing a composition, which is close to an equilibrium composition, is formed.

Joint effect of aluminum, molybdenum and zirconium (β – stabilizers) on the phase composition of the alloys being studied was also calculated for the Ti-Al-V-Mo-Zr system. The fragments of isothermal cuts of the phase diagram of this Ti-system at 800 °C are shown in Figure 2.

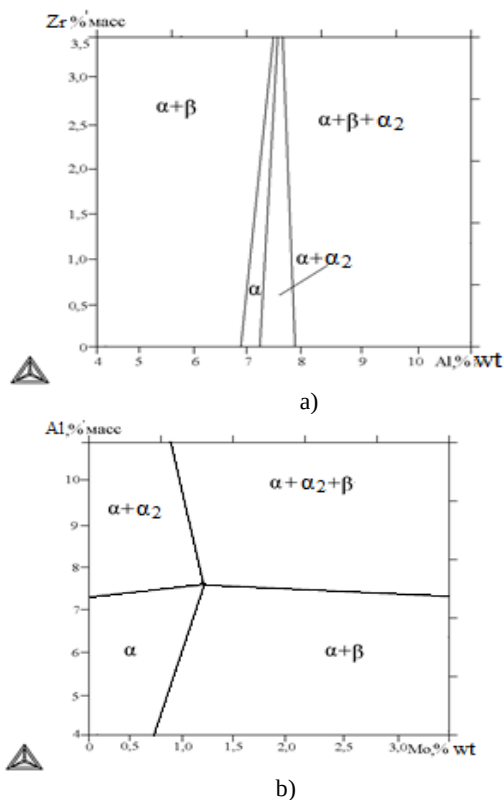


Figure 2 – Fragments of isothermal cuts of phase diagram of Ti-Al-V-Mo-Zr system at 800 °C:
a – 1.3 % V and 1.3% Mo; *b* – 2 % Zr and 1.3 %V

Thermo-Calc program enables the calculation of a huge number of cuts in short time. Making such assessment using the graphical technique is unfeasible for more complicated systems. In this case calculation of the phase composition characteristics at preset concentration of alloying elements and temperatures becomes necessary.

Isothermal cuts at 800 °C make it possible to analyze the joint effect of the two elements Al, Zr and Al, Mo on the

formation of various phases. Calculations show that apart from α and β phases this alloy may contain the intermetallic phase α_2 (Ti_3Al) which is not desirable as its presence leads to a decrease in ductility [5, 6]. Interest here is also generated by the determination of the proportions of excess phases (Q_M) affecting considerably the performance characteristics of castings, which is difficult to perform experimentally. The design values of α and β phases ratio are given in Figure 3.

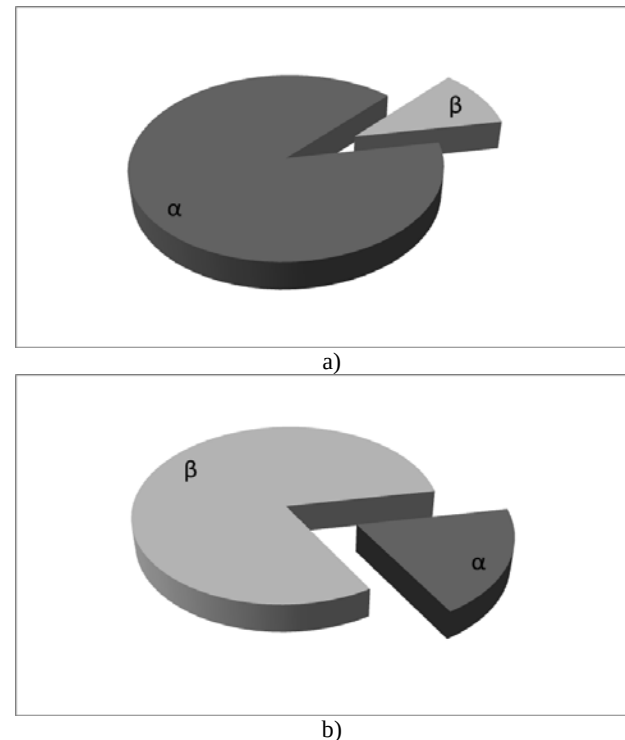


Figure 3 – Design values of α and β phases ratio of Ti-Al-V-Mo-Zr system alloys.
a – 800°C; *b* – 950°C

As indicated in the figure, in the temperature interval from 800 to 950 °C the quantity of β -phase increases by 8 times (from 10 to 80%), which suggests the presence of a phase transition in this temperature region. Based on the above, it was decided that the obtained calculation results shall be checked using experimental samples of the Ti-Al-V-Mo-Zr system alloys containing (%): 6.5 Al, 1 V, 1 Mo, 2 Zr, and annealing at the temperature of 800°C and 950°C.

2.2 Experimental research technique

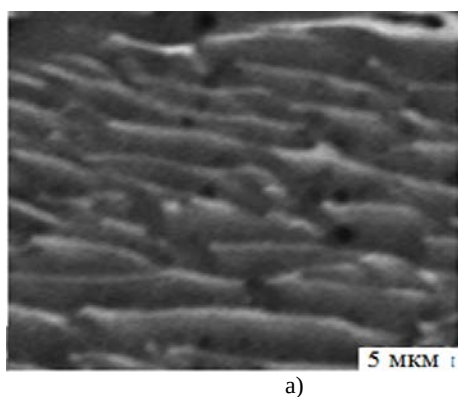
The research subjects were the casting fragments (“corbel” type) of the Ti-Al-V-Mo-Zr system alloy of industrial production. 10x10x15 mm specimens cut from a casting were annealed in a muffle furnace at 800 and 950°C. In order to provide protection from corrosion during annealing, protective coating was applied to the surface of the specimens in accordance with the plasma-electrolytic oxidation process. After holding the specimens were cooled down using two options: cooling in the furnace and quenching in cold water.

The microstructure of the specimens was examined using an optical microscope Axio Observer MAT and electron scanning microscopes (SEM): JSM-6610LV and TESCANVEGA 3. The latter are complete with an energy-dispersive add-on micro-analyzer INCA SDD X-MAX manufactured by Oxford Instruments and software (INCA Energy and Aztec) for microanalysis, construction of composition sections, element distribution maps. The specimens for metallographic research were prepared by means of mechanical

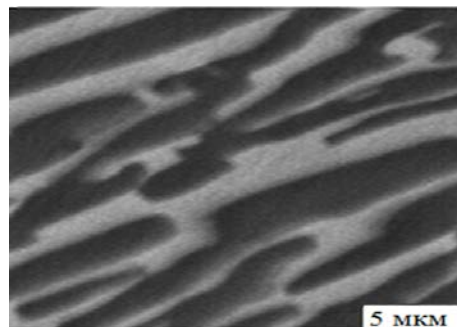
polishing. Polished sections were subjected to chemical etching in a reagent containing 1 ml HF, 1.5 ml HCl, 2.5 ml HNO₃, 95 ml H₂O, during 15 s.

Ti-Al-V-Mo-Zr system alloy structure belongs to the conventional transformed β -type [7] and consists of the α -phase of solid solution of alloying elements and additive agents in titanium with hexagonal close-packed lattice, and of a small quantity of the β -phase of solid solution of alloying elements and additive agents in titanium with bulk-centered lattice.

Titanium alloys are hardened by heat treatment: quenching or ageing. When annealed or quenched they have good ductility, and high strength and resistance to heat after ageing [8, 9]. The more β -phase is contained in the alloy structure, the stronger it is in the as-annealed condition and the more it is hardened during heat treatment. The typical alloy microstructure after heat treatment with different content of additive agents is shown in Figure 3.



a)



b)

Figure 3- Ti-Al-V-Mo-Zr system alloy microstructure after heat treatment;
a) 800°C, b) 950°C

Use of electron scanning microscopes enables more reliable phase identification compared to optical microscopy which does not reveal changes during heat treatment as the phase contrast is due to the difference in atomic numbers. Particularly molybdenum-dressed (the heaviest element in the alloy composition) β -phase looks lighter. Besides due to higher resolving power an electron scanning microscope makes it possible to determine the sizes of the plates having the thickness of less than 1 μ m.

The microstructure of the specimens obtained after annealing at 800°C demonstrates small dark submicron α -phase plates formed during cooling in the process of polymorphic transformation and shaped like colonies and oriented in various directions, as well as a small quantity of β -phase (Fig. 3 a). An increase of up to 950°C in the annealing temperature results in the increase of the size and thickness of the α -plates and their orientation in one direction, as well as increase of the proportion of β -phase (Fig. 3 b).

For the purpose of experimental determination of phase composition several polished sections were analyzed. The results are given in Table 1.

Table 1- Phase composition of the Ti-Al-V-Mo-Zr system alloy under consideration

Components	Component content in phases at temperatures			
	800 °C		950 °C	
	α	β	α	β
Al	6.7	4.9	7.6	6.2
Zr	2.1	2.5	1.7	2.2
Mo	0.8	8.2	0.2	1.8
V	1.4	4.9	0.7	2.0
Ti	89.1	79.5	89.7	87.8

As shown in the table the most significant difference in the distribution between α and β phases is typical for molybdenum and vanadium β -stabilizers. Particularly molybdenum concentration in β -phase decreases from 8.2 to 1.8% as the temperature rises from 800 to 950°C, vanadium – from 4.9 to 2.0%, while the change in zirconium concentration in this phase is insignificant which is due to the fact that zirconium is an analogue of titanium and isomorphically substitutes it in these alloys.

3. Conclusion

Using the Thermo-Calc program isothermal and polythermal cuts of Ti-Al-V-Mo-Zr system were calculated, which enables the assessment of the joint effect of two alloying elements on the phase composition of the alloy being studied.

The conducted research of the structural condition of the Ti-Al-V-Mo-Zr system alloys at various annealing temperatures has shown that within the temperature range of between 800 and 950°C the β -phase content sharply increases to 90%. In the meantime the concentration of β -stabilizing elements Mo and V decreases in both α and β -phases, and the content of aluminium and zirconium (isomorphic analogue of titanium) changes insignificantly.

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WEAR RESISTANCE OF CARBIDE-BAINITE SPHEROIDAL GRAPHITE CAST IRONS UNDER CONDITIONS OF DRY FRICTION

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Abstract: This article presents the outcomes from experimental investigation of the wear resistance of specimens made of carbidic austempered ductile iron (CADI) which are isothermally hardened in the fields of upper and lower bainite. The specimens are subjected of dry friction. A mathematical modeling of the experimental results has been carried out. A regression analysis and analysis of variance (ANOVA) have been fulfilled using QStatLab package. On the basis of the regression models obtained, single-purpose optimization tasks have been solved.

KEYWORDS: CARBIDIC AUSTEMPERED DUCTILE IRON(CADI); WEAR RESISTANCE; OPTIMIZATION.

1. Introduction

Friction and wearing processes take place in the course of interaction between the surfaces of bodies. Therefore, the condition and structure of surfaces exercise decisive influence on the formation of friction forces and wearing mechanism.

Wear resistance is a multi-factor parameter and its forecasting according to properties measured in a standard way (hardness, strength, toughness, etc...) is often wrong. These characteristics are not always reliable criteria for wear resistance of cast irons. The properties of cast irons with spheroidal graphite to withstand against wearing, to a great extent, depend on the structural state, the dimensions of the carbide phase and its distribution. The capability of the latter to break itself into pieces in the matrix thus hardening the surface layer against friction considerably increases wear resistance [1, 2].

The presence of graphite in the structure of ductile irons is of vital importance for their wear behaviour. Under dry friction in single areas of the contact surface practically wearing caused by adhesion is not observed. It is connected with the presence of graphite in the structure which taken alone provides high damping ability and plays the role of a greasing material. When decreasing the distance between the graphite grains, the protective properties of the surface working layer improve and the wear resistance of cast iron increases.

In case of cast irons with metastable structures (retained austenite, martensite, bainite) under conditions of intensive plastic deformation in the area of friction contact, structural transformations that significantly influence the effective strength of the surface, and respectively the wear resistance occur [3].

The purpose of the present research work is to determine the influence of the quantity of carbide phase and the temperature of austempering on the wear resistance of carbide-bainite nodular cast irons under conditions of dry friction.

2. Presentation

To investigate the wear resistance of carbide-bainite nodular cast irons (CBNCI) four compositions with a different content of the carbide phase have been cast (Table 1).

Table 1. Chemical composition of investigated cast irons

№	C, %	Si, %	Mg, %	Quantity of carbide phase, %
1	3,68	2,26	0,028	0
2	3,68	2,22	0,035	9
3	3,63	2,34	0,038	18
4	3,52	2,27	0,025	27

Tests have been carried out on two groups of specimens with a square section (10x10x20 mm), austempered to the mode:

- austenization in a salt bath at 900°C and holding time of 1 hour:

I group - austempered in a salt bath at 300°C with holding time of 90 min and lower bainite structure;

II group - austempered in a salt bath at 400°C with holding time of 60 min and upper bainite structure.

To investigate the wear resistance under dry friction a test stand for accelerated wearing has been used (Figure 1).



Figure 1 Stand for accelerated wear test under dry friction

Wearing is evaluated on the basis of the weight loss upon covering the corresponding distance, respectively time. For every passed hour the absolute mass wearing is calculated and according to ratios 1 and 2 the intensity i and wearing I for each composition and austempering temperature are assessed.

$$i = \frac{\Delta m_i}{\rho \cdot A_a \cdot L} \cdot 10^{-6} \quad (1)$$

where: ρ – material density, $\rho = 7,2 \cdot 10^3 [kg / m^3]$
 A_a - nominal contact surface $A_a = 1 \cdot 10^{-4} [m^2]$
 L - covered distance, respectively time.

$$I = \frac{1}{i} \cdot 10^6 \quad (2)$$

The results of the implemented tests are presented in a tabular and graphic form (Tables 2, 3, 4 and 5 and Figure 2).

Table 2 Influence of the austempering temperature and time of testing on the wear resistance for composition 1

Тем., °C	Маса, г	Време, h / Изминат път L, m							
		1 10598	2 21196	3 31794	4 42392	5 52990	6 63588	7 74186	8 84784
300	m_i	13,0495	13,0059	12,9543	12,9006	12,8515	12,8051	12,7378	12,6889
	Δm_i	0,0425	0,0861	0,1377	0,1914	0,2405	0,2869	0,3542	0,4031
	$i = \Delta m_i / \rho$	5,5697·10 ⁻⁶	5,6418·10 ⁻⁶	6,0153·10 ⁻⁶	6,2708·10 ⁻⁶	6,3036·10 ⁻⁶	6,2665·10 ⁻⁶	6,6312·10 ⁻⁶	6,6034·10 ⁻⁶
	$I = 1 / i$	0,17954·10 ⁶	0,17725·10 ⁶	0,16624·10 ⁶	0,15947·10 ⁶	0,15864·10 ⁶	0,15958·10 ⁶	0,15080·10 ⁶	0,15144·10 ⁶
400	m_i	12,8795	12,7495	12,715	12,6786	12,6242	12,5917	12,5445	12,5051
	Δm_i	0,2146	0,3446	0,3791	0,4155	0,4699	0,5024	0,5496	0,589
	$i = \Delta m_i / \rho$	28,1238·10 ⁻⁶	22,5803·10 ⁻⁶	16,5606·10 ⁻⁶	13,6130·10 ⁻⁶	12,3163·10 ⁻⁶	10,9734·10 ⁻⁶	10,2895·10 ⁻⁶	9,6487·10 ⁻⁶
	$I = 1 / i$	0,03556·10 ⁶	0,04429·10 ⁶	0,06038·10 ⁶	0,07346·10 ⁶	0,08119·10 ⁶	0,09113·10 ⁶	0,09719·10 ⁶	0,10364·10 ⁶

Table 3. Influence of the austempering temperature and time of testing on the wear resistance for composition 2

Тит, °C	Маса, g	Време, h / Изминат път L, m							
		1 10598	2 21196	3 31794	4 42392	5 52990	6 63588	7 74186	8 84784
300	m_0	13,5061	13,4072	13,4096	13,4395	13,4116	13,3667	13,3669	13,3450
	Δm_0	0,0839	0,1028	0,1204	0,1505	0,1784	0,2033	0,2231	0,2450
	$i = \Delta m_0 / \rho A_0 L$	10,9953.10 ⁻⁶	6,7361.10 ⁻⁶	5,2596.10 ⁻⁶	4,9308.10 ⁻⁶	4,6759.10 ⁻⁶	4,4405.10 ⁻⁶	4,1768.10 ⁻⁶	4,0135.10 ⁻⁶
	$I = 1/i$	0,09095.10 ⁶	0,14845.10 ⁶	0,19013.10 ⁶	0,20281.10 ⁶	0,21386.10 ⁶	0,22520.10 ⁶	0,20942.10 ⁶	0,24916.10 ⁶
400	m_0	13,3117	13,2193	13,1557	13,1351	13,0980	13,0763	13,0417	13,0227
	Δm_0	0,1550	0,2474	0,3110	0,3316	0,3687	0,3904	0,4250	0,4440
	$i = \Delta m_0 / \rho A_0 L$	20,3131.10 ⁻⁶	16,2111.10 ⁻⁶	13,5857.10 ⁻⁶	10,8642.10 ⁻⁶	9,6638.10 ⁻⁶	8,5271.10 ⁻⁶	7,9567.10 ⁻⁶	7,2734.10 ⁻⁶
	$I = 1/i$	0,04923.10 ⁶	0,06169.10 ⁶	0,07361.10 ⁶	0,09205.10 ⁶	0,10348.10 ⁶	0,11727.10 ⁶	0,12568.10 ⁶	0,13749.10 ⁶

Table 4. Influence of the austempering temperature and time of testing on the wear resistance for composition 3

Тит, °C	Маса, g	Време, h / Изминат път L, m							
		1 10598	2 21196	3 31794	4 42392	5 52990	6 63588	7 74186	8 84784
300	m_0	13,3041	13,2893	13,2496	13,2478	13,2166	13,1974	13,1787	13,1690
	Δm_0	0,0249	0,0397	0,0794	0,0812	0,1124	0,1316	0,1503	0,1600
	$i = \Delta m_0 / \rho A_0 L$	3,2632.10 ⁻⁶	2,6014.10 ⁻⁶	3,4685.10 ⁻⁶	2,6604.10 ⁻⁶	2,9460.10 ⁻⁶	2,8758.10 ⁻⁶	2,8139.10 ⁻⁶	2,6210.10 ⁻⁶
	$I = 1/i$	0,30645.10 ⁶	0,38441.10 ⁶	0,28831.10 ⁶	0,37589.10 ⁶	0,33944.10 ⁶	0,34773.10 ⁶	0,35538.10 ⁶	0,38153.10 ⁶
400	m_0	13,0988	13,0706	13,0439	13,0170	12,9765	12,9320	12,8955	12,8245
	Δm_0	0,0276	0,0547	0,0825	0,1094	0,1499	0,1944	0,2309	0,3019
	$i = \Delta m_0 / \rho A_0 L$	3,6236.10 ⁻⁶	3,5843.10 ⁻⁶	3,6039.10 ⁻⁶	3,5833.10 ⁻⁶	3,9289.10 ⁻⁶	4,2461.10 ⁻⁶	4,3228.10 ⁻⁶	4,9456.10 ⁻⁶
	$I = 1/i$	0,27597.10 ⁶	0,27900.10 ⁶	0,27747.10 ⁶	0,27907.10 ⁶	0,25452.10 ⁶	0,23551.10 ⁶	0,23133.10 ⁶	0,20220.10 ⁶

Table 5. Influence of the austempering temperature and time of testing on the wear resistance for composition 4

Тит, °C	Маса, g	Време, h / Изминат път L, m							
		1 10598	2 21196	3 31794	4 42392	5 52990	6 63588	7 74186	8 84784
300	m_0	13,8219	13,8038	13,7835	13,7669	13,7556	13,7390	13,7190	13,7010
	Δm_0	0,0171	0,0352	0,0555	0,0721	0,0840	0,1000	0,1200	0,1380
	$i = \Delta m_0 / \rho A_0 L$	2,6606.10 ⁻⁶	2,3098.10 ⁻⁶	2,4266.10 ⁻⁶	2,3639.10 ⁻⁶	2,2030.10 ⁻⁶	2,1853.10 ⁻⁶	2,2462.10 ⁻⁶	2,2606.10 ⁻⁶
	$I = 1/i$	0,44623.10 ⁶	0,43294.10 ⁶	0,41209.10 ⁶	0,42304.10 ⁶	0,45393.10 ⁶	0,45760.10 ⁶	0,44519.10 ⁶	0,44235.10 ⁶
400	m_0	13,9846	13,9546	13,9266	13,9019	13,8752	13,8475	13,8006	13,7525
	Δm_0	0,0200	0,0590	0,0780	0,1027	0,1294	0,1571	0,2040	0,2521
	$i = \Delta m_0 / \rho A_0 L$	2,6210.10 ⁻⁶	3,2763.10 ⁻⁶	3,4074.10 ⁻⁶	3,3648.10 ⁻⁶	3,3916.10 ⁻⁶	3,4314.10 ⁻⁶	3,8192.10 ⁻⁶	4,1298.10 ⁻⁶
	$I = 1/i$	0,38153.10 ⁶	0,30522.10 ⁶	0,29348.10 ⁶	0,29720.10 ⁶	0,29484.10 ⁶	0,29143.10 ⁶	0,26183.10 ⁶	0,24214.10 ⁶

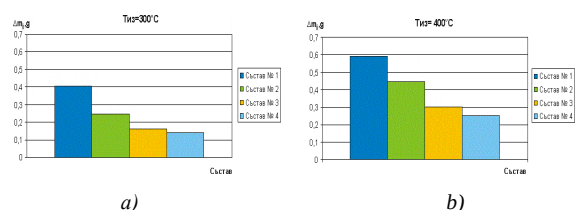


Figure 2. Loss of mass at times of testing of 8 hours for samples austempered at a) 300°C and b) 400°C

To do a quantitative and qualitative analysis, a regression and variance analysis is carried out by means of a QStatLab system, using the results obtained from the planned experiment [4, 5].

The plan of the experiment, the controlling factors and their levels of variation for the target function Y_3 are presented in Tables 6 and 7.

Table 6. Controlling factors and their levels

Управляващи фактори		Нива на факторите							
u_1	Време, h	Натурални	1	2	3	4	5	6	7
		Кодирани	-1	-	-	-	+	+	+
u_2	Карбидна фаза $\phi_{K\phi}$, %	Натурални	0	9	18	27			
		Кодирани	-1	-0,333	+0,333	+1			
u_3	Температура на изотермично закаляване $T_{из}$, °C	Натурални	300	400					
		Кодирани	-1	+1					

Controlling factors - Управляващи фактори ; Time-Време; Carbide phase-Карбидна фаза; Levels of factors-Нива на факторите; Austempering Temperature-Температура на изотермично закаляване; Natural-Натурални; Coded-Кодирани.

Table 7 Plan of the experiment and results for Y_3

№	u_1	u_2	u_3	$Y_3 \cdot 10^6$
1	-1	-1	-1	0,17954
2	-0,714	-1	-1	0,17725
3	-0,429	-1	-1	0,16624
4	-0,143	-1	-1	0,15947
5	+0,143	-1	-1	0,15863
6	+0,429	-1	-1	0,15958
7	+0,714	-1	-1	0,15080
8	+1	-1	-1	0,15144
9	-1	-1	+1	0,03556
10	-0,714	-1	+1	0,04429
11	-0,429	-1	+1	0,06038
12	-0,143	-1	+1	0,07346
13	+0,143	-1	+1	0,08119
14	+0,429	-1	+1	0,09113
15	+0,714	-1	+1	0,09719
16	+1	-1	+1	0,10364
17	-1	-0,333	-1	0,09095
18	-0,714	-0,333	-1	0,14845
19	-0,429	-0,333	-1	0,19013
20	-0,143	-0,333	-1	0,20281
21	+0,143	-0,333	-1	0,21386
22	+0,429	-0,333	-1	0,22520
23	+0,714	-0,333	-1	0,20942
24	+1	-0,333	-1	0,24916
25	-1	-0,333	+1	0,04923
26	-0,714	-0,333	+1	0,06169
27	-0,429	-0,333	+1	0,07361
28	-0,143	-0,333	+1	0,09205
29	+0,143	-0,333	+1	0,10348
30	+0,429	-0,333	+1	0,11727
31	+0,714	-0,333	+1	0,12568
32	+1	-0,333	+1	0,13749
33	-1	+0,333	-1	0,30645
34	-0,714	+0,333	-1	0,38441
35	-0,429	+0,333	-1	0,28831
36	-0,143	+0,333	-1	0,37589
37	+0,143	+0,333	-1	0,33944
38	+0,429	+0,333	-1	0,34773
39	+0,714	+0,333	-1	0,35538
40	+1	+0,333	-1	0,38153
41	-1	+0,333	+1	0,27597
42	-0,714	+0,333	+1	0,27900
43	-0,429	+0,333	+1	0,27747
44	-0,143	+0,333	+1	0,27907
45	+0,143	+0,333	+1	0,25452
46	+0,429	+0,333	+1	0,23551
47	+0,714	+0,333	+1	0,23133
48	+1	+0,333	+1	0,20220
49	-1	+1	-1	0,44623
50	-0,714	+1	-1	0,43294
51	-0,429	+1	-1	0,41209
52	-0,143	+1	-1	0,42304
53	+0,143	+1	-1	0,45393
54	+0,429	+1	-1	0,45760
55	+0,714	+1	-1	0,44519
56	+1	+1	-1	0,44235
57	-1	+1	+1	0,38153
58	-0,714	+1	+1	0,30522
59	-0,429	+1	+1	0,29348
60	-0,143	+1	+1	0,29720
61	+0,143	+1	+1	0,29484
62	+0,429	+1	+1	0,29143
63	+0,714	+1	+1	0,26183
64	+1	+1	+1	0,24214

From the performed regression analysis the following model is obtained for the target function Y_3 :

$$Y_3 = 0,228 + 0,027u_1 + 0,251u_2 - 0,046u_3 - 0,020u_1^2 + 0,013u_2^2 - 0,126u_3^2 - 0,081u_1u_2 - 0,012u_2u_3 - 0,032u_1u_2^2 - 0,027u_1u_2u_3 - 0,012u_2^2u_3 - 0,029u_1^3u_2 - 0,025u_1^3u_3 + 0,025u_1^2u_2^2 + 0,088u_1u_2^3 + 0,016u_1u_2^2u_3 \quad (3)$$

In Figures 3 and 4 the diagrams of the main effects of the controlling factors and the graphic interpretation of the influence of the three factors on the wear resistance according to the section method are presented.

The results for the analyzed range of variation could be summarized as follows:

- From the three analyzed factors the influence of the percentage content of the carbide phase, (u_2) is the highest, austempering temperature is the second highest, (u_3), time exercises the least influence, h (Figure 3);
- The percentage content of the carbide phase influences the utmost extent the wear resistance when u_2 is within the range $(0 \div 1)$;
- To achieve higher wear resistance it is advisable to apply austempering at a temperature of 300 °C.

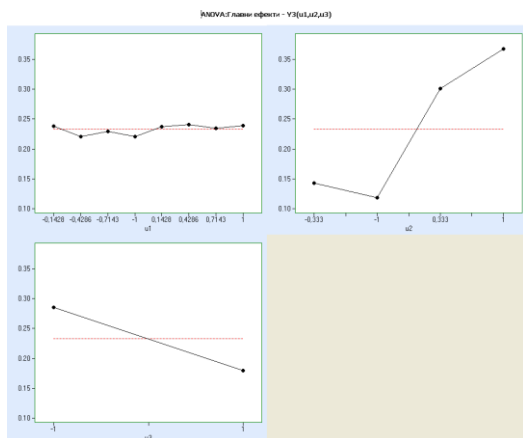


Figure 3 Main effects of the controlling factors on the function Y3

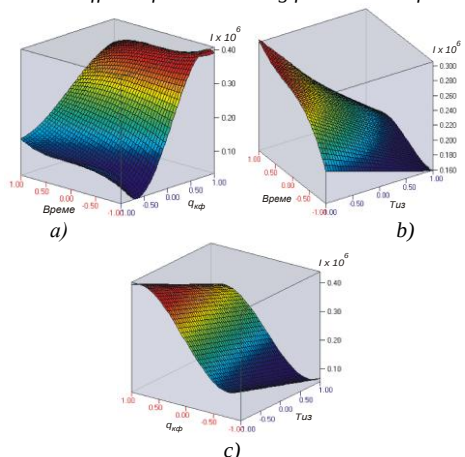


Figure 4 Influence of the factors on the wear resistance under dry friction

The main purpose of optimization is to determine what combination of the values of the controlling factors will provide the highest wear resistance. For this purpose the following one-target optimization task is solved:

- Determination of the optimum values of the factors u_1 , u_2 и u_3 at which the wear resistance under dry friction is maximum.

The optimization task is based on the obtained regression model (3). The obtained optimum values of the controlling factors that provide maximum wear resistance are shown in Table 8.

Table 8. Optimum values of the controlling factors for which Y3 is maximum

u_1	Time h	Coded	1
		Natural	8
u_2	Amount of carbide phase $q_{kf}, \%$	Coded	1
		Natural	27
u_3	Austempering temperature $T_{u3}, ^\circ C$	Coded	-1
		Natural	300

3. Conclusions

The influence of the amount of carbide phase on the wear resistance of carbide-bainite nodular cast irons austempered in the area of lower and upper bainite has been investigated.

It is established that if there are equal amounts of carbide phase, cast irons with a lower bainite structure of the metal matrix obtained at austempering temperature of 300°C have higher wear resistance.

A regression model of wear resistance of CBNCI based on a planned experiment has been obtained.

A variance analysis for quantitative evaluation of the influence of the controlling factors on the wear resistance under dry friction of the examined CBNCI compositions has been done.

From the implemented one-target optimization of the wear resistance under conditions of dry friction it has been established that in order to provide maximum wear resistance it is advisable to use CBN cast irons of 27 % content of carbide phase, austempered in the area of lower bainite at an austempering temperature of 300°C.

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GRADIENT INTERFERENCE OPTICAL FILTERS MANUFACTURED FROM ORGANOSILICONE COMPOUNDS WITH THE RF PECVD TECHNIQUE

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Abstract: Chemical structure and optical properties of thin coatings synthesized from organosilicone precursors by means of radio frequency plasma enhanced chemical vapor deposition were studied by means of Fourier transform infrared spectroscopy, scanning electron microscopy and variable angle spectroscopic ellipsometry. Both precursors, namely hexamethyldisilazane (HMDSA) and tetramethyldisilazane (TMDSA) were used to deposit films under conditions of different proportions of oxygen to nitrogen in the reaction mixture. In both cases, changing that proportion from 0% to 100% resulted in a substantial change of refractive index of the resulting coating, from 2.22 to 1.65 and from 2.31 to 2.03 for HMDSA and TMDSA, respectively. The results obtained allowed us to design and to manufacture a “rugate” interference optical filter with a gradient value of refractive index. For that purpose, HMDSA precursor was selected as one enabling a change of refractive index in a much broader range.

KEYWORDS: HMDS, TMDS, CVD, INDEX OF REFRACTION, GRADIENT FILTERS, STRUCTURE

1. Introduction

Due to their physical and chemical properties, thin amorphous $\text{Si}_x\text{O}_y\text{N}_z\text{:C}$ coatings have variety of applications. They are characterized by low absorption losses in the visible and near infrared regions. Their index of refraction may be easily controlled within the range of 1.45 ($\text{Si}_x\text{O}_y\text{:C}$) and 2.2 ($\text{Si}_x\text{N}_z\text{:C}$) [1]. Therefore, these coatings are often utilized in optoelectronics, for instance in lightguides [2,3] and in photovoltaics [4]. In a photovoltaic cell, a coating with variable refractive index enhances its effectiveness by increasing the amount of radiation absorbed [5,6]. In VLSI circuits, it may serve as a dielectric or passivation film and, in CMOS VLSI, it is used to control the threshold voltage of a MOS device [7-9].

A potential to change optical properties of $\text{Si}_x\text{O}_y\text{N}_z\text{:C}$ coatings produces a number of application opportunities, among others, in a construction of the so called “rugate” interference optical filters, i.e. filters with a continuous change of their index of refraction. Such devices are characterized by sinusoidal refractive index dependence on the distance from the substrate [10,11]. This is a reason why, a photonic forbidden gap, similar to that present in a Bragg mirror may be found in these filters. For gradient filters, the index of refraction may be presented by the following formula [12]:

$$n(x) = n_a + \frac{1}{2} n_p \cdot \sin\left(\frac{4\pi x}{\lambda_0} + \phi_0\right)$$

where x denotes optical path, n_a denotes mean refractive index, n_p denotes difference between high and low refractive index (kontrast coefficient), λ_0 denotes a wavelength for the gap and ϕ_0 denotes initial phase.

When high order maxima begin to appear in a low amplitude profile, a sinusoidal logarithm of an index of refraction should be used, described by the following formula:

$$\log[n(x)] = \frac{\log n_H + \log n_L}{2} + \frac{\log n_H - \log n_L}{2} \cdot \sin\left(\frac{4\pi x}{\lambda_0}\right)$$

where n_H , n_L denote high and low index of refraction.

In order to eliminate imperfections, in the transmission spectrum emerging at the edges of the gap, one can introduce a soft change of a contrast coefficient n_p at the film boundaries. This should to a large extend eliminate interference fringes and stabilize a transmission spectrum.

Optical filters of such a construction are narrow-band devices, allowing one to retain very high optical efficiency, by lowering losses connected with interference scattering and suppression of high order harmonic components. In should be emphasized here that a proper filter design should provide its antireflection performance within a broad visible range. In addition, such filters

exhibit lower sensitivity to the angle of incidence and are characterized by higher mechanical strength.

The present work is devoted to a comparison of optical coatings produced by means of radio frequency plasma enhanced chemical vapor deposition (RF PECVD) method from two different organosilicone precursors, namely hexamethyldisilazane (HMDSA) and tetramethyldisilazane (TMDSA), under conditions of varying content of oxygen in the reaction mixture. The effect of that content on the films structure, morphology and optical properties will be studied with the help of such analytical techniques as scanning electron microscopy (SEM), Fourier transform infrared (FTIR) spectroscopy and variable angle spectroscopic ellipsometry (VASE) techniques. In addition, the work will also present optical coatings characterized by a gradient change of refractive index.

2. Experimental

A schematic view of the RF PECVD reactor used in this work is presented in **Figure 1**. The main part of that reactor is comprised of a reaction chamber equipped with a water-cooled RF electrode, with the chamber walls playing the role of the counterelectrode. The substrates are placed on the RF electrode. Two distribution lines, one for gaseous media and one for liquid precursor compounds, supply material to the reactor. The liquid precursor compound comprise Sigma Aldrich HMDSA of a purity 99% and Sigma Aldrich TMDSA of a purity 97% while the gaseous media comprise Linde Gas Polska oxygen of a purity 99.999% and comprise Linde Gas Polska nitrogen of the same purity. The flow rates of both gases are regulated by the mass flow controllers, with the flow rates of vaporized liquid precursors controlled by bubbler temperatures 40°.

All the deposition processes were carried out at one of the three compositions of the gas phase. One was 100% of nitrogen, one was 50% of nitrogen and 50% of oxygen and one was 100% of oxygen. The remaining parameters of the deposition processes were kept constant and they were as following: total flow rate of the gas medium equal 30 SCCM, system pressure equal 45 Pa.

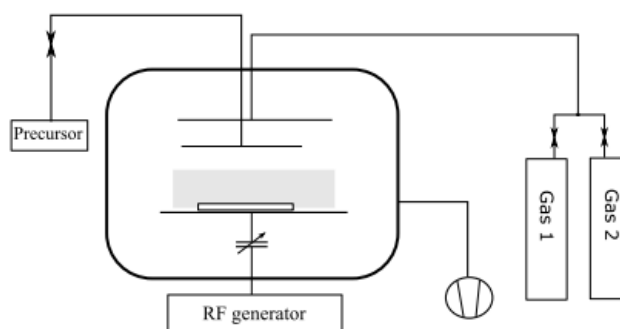


Fig. 1 Schematic representation of the RF PECVD system

Both optical properties and the thickness of the films were determined with the help of J.A. Woollam VASE ellipsometer working at three different values of the angle of incidence equal 65°, 70° and 75°. The measurements were performed within the spectral range of 260 nm to 1000 nm, with the measurement step equal 5nm.

Film surface images were recorded with the JEOL JSM-6610LV scanning electron microscope integrated with the MiniCL-GATAN Cathodoluminescence Imaging system, Oxford Instruments EDS X-MAX 80 system and EBSD NordlysMax back-scattered electron acquisition detector.

FTIR analysis was carried out within the measurement range of 4000 to 500 cm^{-1} , with the resolution of 4 cm^{-1} using ThermoScientific Nicolet iS50 FTIR spectrometer equipped with the DTGS KBr beam splitter. The measurements were performed in the absorbance mode with the number of scans for one cycle amounting 64.

3. Results and discussion

The coatings synthesized from both HMDSA and TMDSA precursors at different contents of oxygen in the reaction mixture were examined, with regard to the structure of their chemical bonds, by means of FTIR spectroscopy. The results are presented in **Figures 2 and 3**, respectively for HMDSA and TMDSA precursors, each at three different proportions of nitrogen to oxygen. As seen in both figures, a formation of Si-O bonds on the expense of Si-C and Si-N bonding takes place along with an increasing oxygen content in the reaction mixture. All the three bonds presented above are responsible for the numerical values of such optical properties of the material as index of refraction and extinction coefficient. A change of proportions between these bonds, resulting from the increasing concentration of oxygen in the reaction mixture, reveals a transformation of the material chemical structure from that of silicon carbonitride to that of silicon carboxide. This, in turn, gives one an opportunity to arrive at the predetermined magnitude of refractive index, remaining in the range between the lowest and the highest value obtainable under particular experimental conditions. In parallel, the increasing amount of oxygen in the reaction mixture reduces a number of C-H bonds and brings about an increase of the content of C-O bonds.

A detailed analysis of FTIR spectra presented in **Figures 2 and 3**, shows that the chemical structure of the coatings prepared from HMDSA undergoes faster and more evident transformation than that of the films synthesized from TMDSA. Therefore, from the point of view of a synthesis of gradient optical coatings, HMDSA appears to be a better selection of an organosilicone deposition precursor than TMDSA.

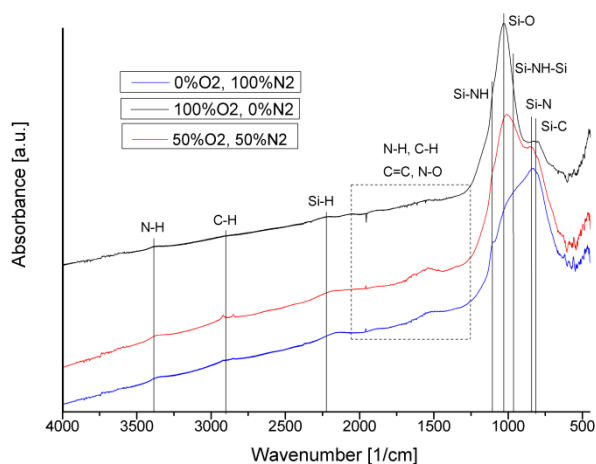


Fig. 2 FTIR evidence of chemical structure of the coatings deposited from HMDSA at different proportions of nitrogen to oxygen

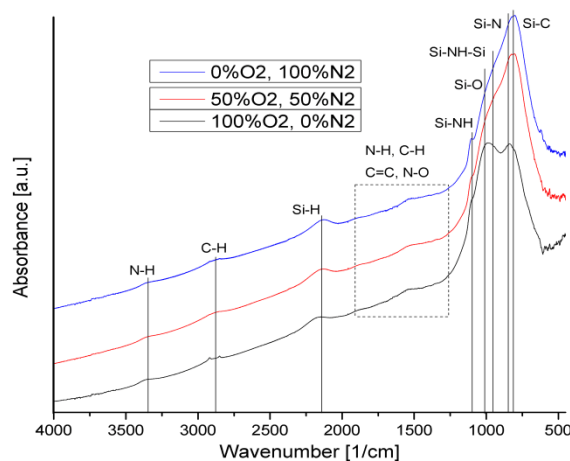


Fig. 3 FTIR evidence of chemical structure of the coatings deposited from TMDSA at different proportions of nitrogen to oxygen

SEM images presented in **Figure 4** show that the coatings synthesized from both HMDSA and TMDSA precursors are homogeneous and free of surface defects.

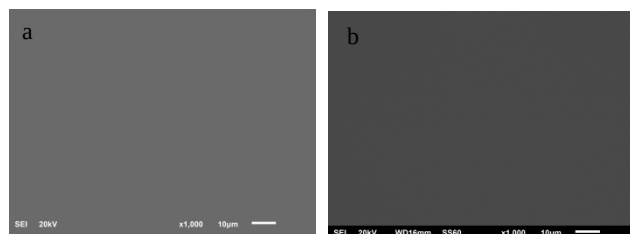


Fig. 4 SEM images of the coatings deposited from HMDSA (a) and TMDSA (b) precursors

Optical constants of the coatings were determined by means of a measurement of a polarization ellipse of a reflected light. An application of a Couche model allowed us to compute three essential parameters of the films, their thickness as well as refractive index and extinction coefficient at the wavelength of 550 nm. The results are presented in **Table 1**.

As seen in the table, an increasing oxygen content in the reaction mixture during the deposition brings about a lowering of refractive index in the resulting coating. This effect is more pronounced for the coatings synthesized from the HMDSA precursor, for which the magnitude of refractive index varies within the range of 1.65 to 2.22. In contrast, the coatings deposited from TMDSA are characterized by a substantially lower span of change, remaining between 2.0 and 2.3

Taking into account all the results presented, one can state that oxygen is more easily incorporated into the structure of the coatings synthesized from HMDSA than into that deposited from TMDSA. This gives the former process a better opportunity to control an index of refraction in the wider range and, therefore, to manufacture more efficient “rugate” interference filters with a gradient of this parameter. As far as the magnitudes of extinction coefficient are concerned, they vary between 0.02 to 0.04 and between 0.01 and 0.05, for the films deposited from HMDSA and TMDSA, respectively. These are relatively large values and they very likely result from a presence of carbon in the coatings. There is a number of publications describing a relationship between optical parameters of the films and their chemical bonding. Jędrzejewski et al. [13], for instance, argue in their work that the value of refractive index of silicon carbonitride coatings strongly depends on a non-equilibrium content of such bonds as: Si-C ($n=2.5$), Si-N ($n=1.85$) and C-N ($n=2.6$). These bonds are primarily responsible for the high refractive index of the coatings deposited under conditions of an absence of oxygen in the reaction mixture.

Tab. 1 Ellipsometric data of the coatings synthesized from HMDS and from TMDS at different proportions of oxygen to nitrogen in the reaction mixture.

		HMDS		
N ₂	O ₂	d [nm]	n	k
100%	0%	169,08	2,22	0,04
50%	50%	144,08	1,92	0,02
0%	100%	135,81	1,65	0,02
		TMDS		
N ₂	O ₂	d [nm]	n	k
100%	0%	309,64	2,31	0,01
50%	50%	230,00	2,13	0,02
0%	100%	251,22	2,03	0,05

Based on information acquired from the above data, it became possible to manufacture a gradient interference filter with a continuous change of an index of refraction from high to low magnitude. The results of a VASE investigation of such a filter are presented in **Figure 5** below.

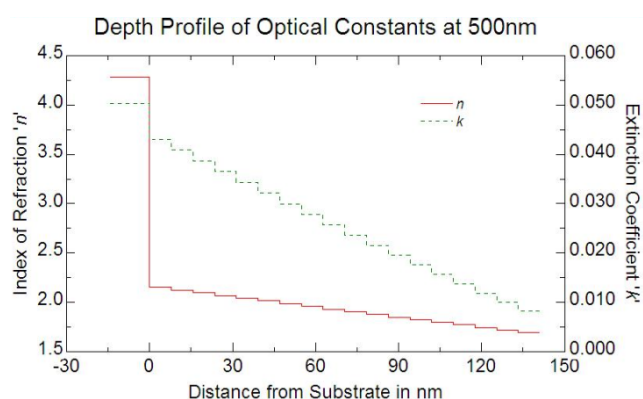


Fig. 5 Results of VASE ellipsometric characterization of a gradient interference filter, deposited from HMDSA on a silicon substrate, characterized by a single transformation from a high to a low magnitude of refractive index

As seen in the figure, the structure and, therefore, optical properties of the filter change in a function of its thickness. With a continuous change of oxygen content in the reaction mixture from 0% to 100%, the magnitude of refractive index changes from approximately 2.2 to approximately 1.6.

4. Conclusion

The results presented show that it is possible to manufacture “rugate” interference optical filters equipped with a gradient of refractive index by means of RF PECVD deposition from organosilicone precursors at continuously varying proportion of oxygen to nitrogen in the reaction mixture. Out of the two precursors tested in the work, HMDSA turned out substantially better, allowing to change a magnitude of refractive index within a relatively broad range between 1.65 and 2.22.

Acknowledgements

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