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Nano, Bio, Green and Space:
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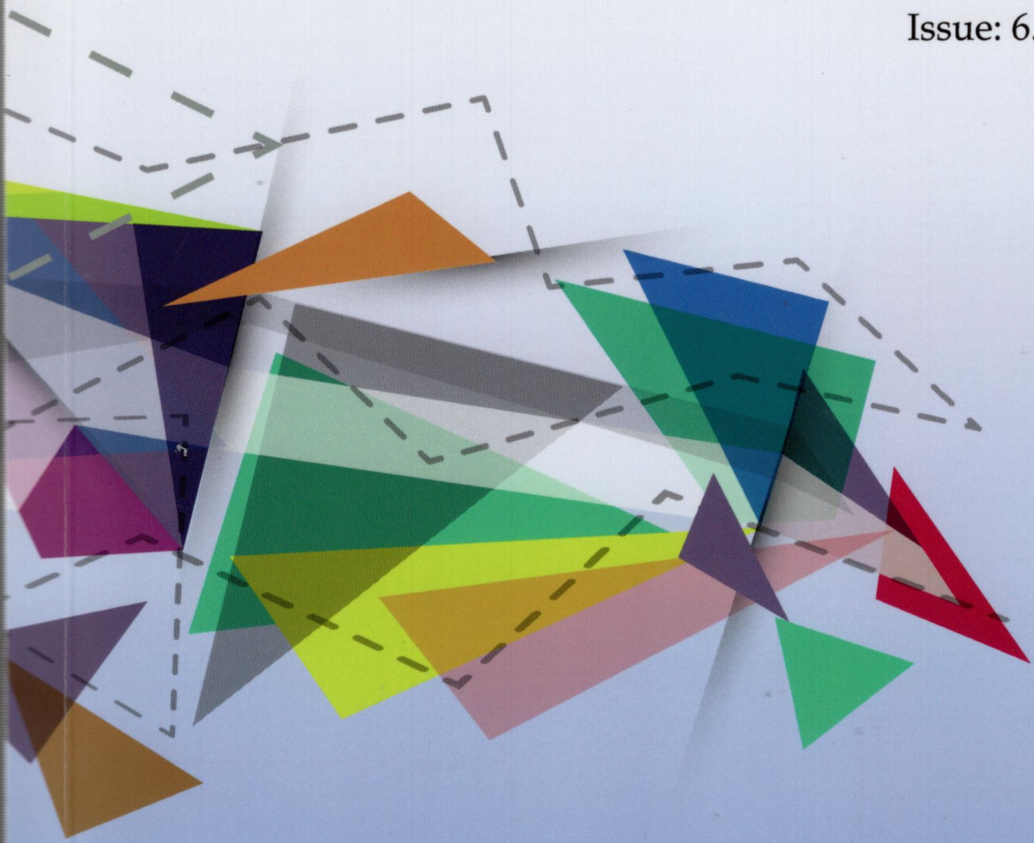

MICRO AND NANO TECHNOLOGIES
ADVANCES IN BIOTECHNOLOGY

CONCLUSION

Energetic analysis points out only the energy losses transferred to the external medium. It cannot make any qualitative difference between different kinds of energies.

For the hot water boiler only the 10% loss ($\varphi_{L\,WB}$ =0.1 or η_{WB}=0.9) due to incomplete insulation leads to an energetic performance COP_{en}=0.9 and not unitary.

On the other side, from the energetic point of view, the thermal energy conversion into mechanical work (electrical energy) seems to be the less performing. For the low energetic efficiency of the steam turbine installation COP_{en}^{el}=0.27, the energetic analysis find guilty the condenser whose loss is 63% from the installation energy input.

Only the exergetic analysis can give information about the way in which the potential of an energy to do something useful is destroyed. For the exergetic analysis the condenser brings an insignificant destruction due to the low temperature level, close to the environmental one of the heat rejected into the environment.

The true cause of inefficiency in the steam turbine installation is the combustion process and heat transfer across a large temperature difference in the steam generator that destroys 61% from the consumed fuel.

When producing separately heat and power two main exergy destruction appear in the two combustion processes.

As expected the cogeneration of heat and electrical energy by eliminating one combustion process and the use of the low pressure steam (low exergy) for producing hot water leads to the highest exergetic efficiency COP_{ex}^{Co} =30%

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COMPARISON OF ANTIDIABETIC EFFECTS OF *P. SONCHIFOLIA*, *C. ROSEUS* AND *M. CHARANTIA* EXTRACTS AND GREEN SYNTHETIZED ZNO NANOPARTICLES TOWARDS COMMON CARP MODEL: *IN VITRO* STUDY

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ABSTRACT

The global burden of diabetes has elevated significantly during last decades. It has highly been appreciated that appropriate animal models that familiarly resemble the hyperglycemia and type 2 diabetes are urgently needed for understanding and seeking of concepts cover biochemical and molecular *mechanism* implicated early in the development and *progression* of the disease. To this purpose we studied the response of *Cyprinus carpio* red blood cells (RBC) to high glucose exposure *in vitro* and potentials of medicinal herbs (*Polymnia (Smallanthus) sonchifolia, Catharanthus roseus, Momordica charantia*) and zinc-containing compounds against glucose toxicity.

The results have shown that the glucose treatment was capable to cause the oxidative stress, and enhance the rate of hemolysis. When glucose-treated RBC were probed with tested compounds, specific response to different co-exposures, but similar to compatible compounds was disclosed. Zinc picolinate in general had no effect on the studied parameters except of TBARS and hemolysis, then ZnO nanoparticles made glucose effects more profound. *P. sonchifolia* didn't provoke significant variation of investigated parameters with one exception when compared to glucose-treated cells. *Momordica* which is well-known nutraceutical with metabolic and antiglycemic effects and tested *Catharanthus roseus* both in herbal extract form and green synthetized ZnO nanoparticle have caused the decreased in TBARS and rate of hemolysis, and the increased in catalase and glutathione up to control baseline. These results have pointed to the necessity of further investigations of antihyperglycemic activity of *Momordica* and *Catharanthus* and mechanistic explanation of their potentials.

Keywords: *Catharanthus roseus, Momordica charantia,* green synthetized ZnO nanoparticle, oxidative stress, hemolysis

INTRODUCTION

The number of patients with endocrinopathies, primarily diabetes mellitus and obesity, is steadily increasing throughout the world. According to WHO (who.int), in January 2010, there were 285 million patients with diabetes, and by the year 2030 their number

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could reach 438 million [1]. At the same time, the main share of the people suffered from diabetes belongs to the people (more than 90%) with type 2 diabetes (T2D). Currently, 80% of the world population with diabetes lives in low-income countries and countries with transition economies [1]. 1.2 million patients with diabetes have been registered in Ukraine in 2016 (moz.gov.ua). The amount of people with diabetes and those with undiagnosed and uncontrolled hyperglycemia in the developing countries is rapidly increasing and finally forms the background for further investigation (www.who.int), detailed study of the biochemical and molecular mechanisms that determine the early development and progression of the disease, the pathogenesis of diabetes complications and the development of new approaches to their treatment. Hence, there is an urgent need to find convenient, alternative animal models that mimic T2D and contribute to a better understanding of approaches to the detection of glycemic states and diabetes, their complications, and can also be used to test new drugs for the treatment of endocrine pathologies.

Zinc is essential element important for numerous peptides and proteins synthesis, among them insulin as well as carbohydrate metabolism [2]. It has shown that diabetes is come along hypozinkemia and hyperzincuria, and zinc supplementation provides some benefits in patients and rodents with diabetes namely regulation of fasting insulin levels and fasting blood sugar [3]. The alternative natural supplement with potential antihyperglycemic effect is represented by medicinal plants. They can improve the operating rate of the pancreas, which is achieved by intensification insulin secretion or decreasing the intestinal absorption of glucose. Unfortunately, not too much is known about combine effects of zinc and herbs on diabetes and its complications [4], [5].

Hyperglycemia and diabetes arrange "ideal" conditions for the formation of oxidative stress: the content of oxidation substrates (glucose and lipids) free radicals formation are elevated and / or the activity of antioxidant defense systems decreases [6], [7]. Oxidative stress is considered as a "universal basis" for the development of diabetes complications stimulated by the endothelial dysfunction and damage of β-cells in particular [7]. In our previous studies, we have estimated that after glucose treatment of fish *in vivo* signs of oxidative damage and / or uncompensated suppression of stress systems, accompanied by manifestations of cytotoxicity and genotoxicity, are developed [8]. The present study reports new green synthetized ZnO nanoparticles based on medicinal herbs (*Polymnia (Smallanthus) sonchifolia, Catharanthus roseus* and *Momordica charantia*). These formula's anti-diabetic molecular mechanisms were demonstrated in *Cyprinus carpio* cell models.

METHODS AND MATERIALS

Animal maintenance and cell isolation

The experiments were carried out in December of 2018. Adult specimens of common carp *Cyprinus carpio* (17–19 cm long and 270–320 g weight) were collected from a fish farm located in a reference site where no source of contamination is registered. Fish were delivered to the laboratory in 50 L cages with aerated native water. Experiments were performed in accordance with the national and institutional guidelines for the protection of animal welfare and approval of the Committee on the Bio-Ethics at Ternopil V. Hnatiuk National Pedagogical University (No 3/03.12.2018). After 7 days of acclimation to laboratory conditions, the fish were anesthetized with clove oil, the

whole blood was collected from the heart, and red blood cells (RBC) were immediately separated by gradient centrifugation of the whole blood at 1000 ×*g* for 15 min. RBCs were collected from the pellet. After careful removal of the leukocytes, RBC were resuspended to a final hematocrit of 10% in the sterile incubation medium (90.5 mM NaCl, 3 mM KCl, 1.3 mM $CaCl_2$, 0.5 mM $MgSO_4$, 5 mM glucose, 1 mM pyruvate, 1 mM Tris-HCl, pH = 7.4) with amino acids and gentamicin sulphate.

Experimental design

The putative effect of zinc picolinate (77 µmol), manufactured ZnO nanoparticles (Sigma) (77 µmol), herbal extracts (leaf extract of *Polymnia (Smallanthus) sonchifolia* and *Catharanthus roseus* and fruits extract of *Momordica charantia)* and synthetized (by means of green-synthesis technology) ZnO-herbal complexes were evaluated in common carp RBC in terms of their antihyperglycemic activity. RBC incubated at 20 °C for 48 h with continuous mixing. Control was constituted of RBC in 5 mM glucose, but not exposed to any zinc-containing substances and herbal extracts. Experimental groups were constituted of RBC in 40 mM glucose, and simultaneously exposed to zinc-containing substances and herbal extracts. The studied glucose concentration was in the range had been applied in earlier studies by other authors [9]. RBC and the incubation medium of all coarse dispersion with additives were segregate by centrifugation at 1500 × g for 10 min.

Green-synthesis technology

Green synthesis of ZnO nanoparticles using a leaf extract of *Polymnia (Smallanthus) sonchifolia* and *Catharanthus roseus* and fruits of *Momordica charantia* carried out from $ZnSO_4$ solution. For synthesis of nanoparticles, 25 ml of 2.25% plant extract was taken and heated to 60-80°C. Then a 10% solution containing 2.5 g of zinc sulphate was added and the mixture was boiled until it diminished to dark-yellow paste. This paste was then collected in a ceramic mortar and heated at 200 °C for 2 minutes [10]. The resulting light yellow powder was used for exposure.

All protocols were used for analytical measurements represent in detailed in [11].

Oxidative stress parameters

Catalase (CAT, EC 1.11.1.6) activity was measured in a hemolysate by evaluating the decomposition of 10 mM H_2O_2 according to Aebi (1974) at 240 nm ($\varepsilon = 40\ M^{-1}\ cm^{-1}$) in a medium containing 50 mM KH_2PO_4 (pH 7.0) and approximately 150 µg of proteins. Enzyme activity was expressed as µmol per g of Hb.

Lipid peroxidation (LPO) was determined in a hemolysate after trichloroacetic acid treatment in the final concentration of 30% by the production of TBA-reactive substances (TBARS) (Ohkawa et al., 1979). The absorbance of the chromogen was determined at 532 nm. A molar extinction coefficient of $1.56 \cdot 10^5\ M^{-1}\ cm^{-1}$ was used. Data were expressed as nmol TBARS g^{-1} Hb.

Protein carbonyl (PC) concentration, as an index of protein damage, was measured in the pellet of the trichloroacetic acid-treated hemolysate by the reaction with 2,4-dinitrophenylhydrazine (DNPH) (Reznick and Packer, 1994). Differences in the absorbance between the DNPH- and the HCl-treated samples were determined spectrophotometrically at 370 nm, and the concentration of carbonyls was determined

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by using a molar extinction coefficient of $2.2 \cdot 10^4$ M^{-1} cm^{-1}. Data were expressed as nmol PC g^{-1} Hb.

Total glutathione (GSH) concentration in RBC lysate after proteins precipitation with sulfosalicylic acid (5%) was quantified by the glutathione reductase recycling assay (Anderson, 1985). Standards were prepared from the reduced glutathione (GSH), and concentrations were presented as μmol per g Hb. The rate of 5-thionitrobenzoic acid formation was monitored spectrometrically at 412 nm. Standards were prepared from reduced glutathione (GSH), and concentrations were expressed as μmol per g^{-1} Hb.

Hemolysis assay

After exposure, the RBC samples were centrifuged (5000g, 10 min) and Hb concentration in the supernatant was registered at 540 nm. A value of 100% lysis was stated to the supernatant of the sample with control hemolysate, obtained by freezing and thawing the RBC dispersion. The rate of hemolysis in tested samples was calculated related to the sample with control hemolysate [9].

Hemoglobin in RBC lysates was estimated by cyanomethemoglobin method using Drabkins reagent.

Statistical analysis

Statistical analyses were performed on raw data using the Statistica 12.0 software (StatSoft, USA). Data were tested for normality and homogeneity of variance by Kolmogorov-Smirnoff and Levene's testsand normalized whenever possible by Box-Cox common transforming method. The effects of tested compounds on the selected biological traits were analyzed by one-way ANOVA. Pearson's correlation test was used to assess correlations between the studied traits. $p<0.05$ was considered as significant. The data are presented as means ± standard deviation (SD) unless indicated otherwise.

RESULTS AND DISCUSSION

The exposure of carp RBC with glucose caused a substantial ($p < 0.05$) increase in TBARS (by 56%), but a decrease in catalase activity (by -51%) and particularly in total glutathione concentration (by -77%). Co-treatment of RBC with zinc in picolinate and nanoform disclosed different effects on glucose-treated RBC. When zinc picolinate didn't provoke significant changes in studied traits, ZnO deepened changes induced by glucose videlicet stimulation of lipid and protein oxidation and oppression of catalase and glutathione (Fig. 1). *P. sonchifolia* didn't provoke significant variation of investigated parameters with one exception when compared to glucose-treated cells. Meantime *Momordica* which is well-known nutraceutical with metabolic and antiglycemic effects and tested *Catharanthus roseus* both in herbal extract and ZnO-herbal complex have protected RBC from lipid and protein oxidation induced by glucose, highly likely via stimulation of antioxidants namely catalase and glutathione which came back to control baseline.

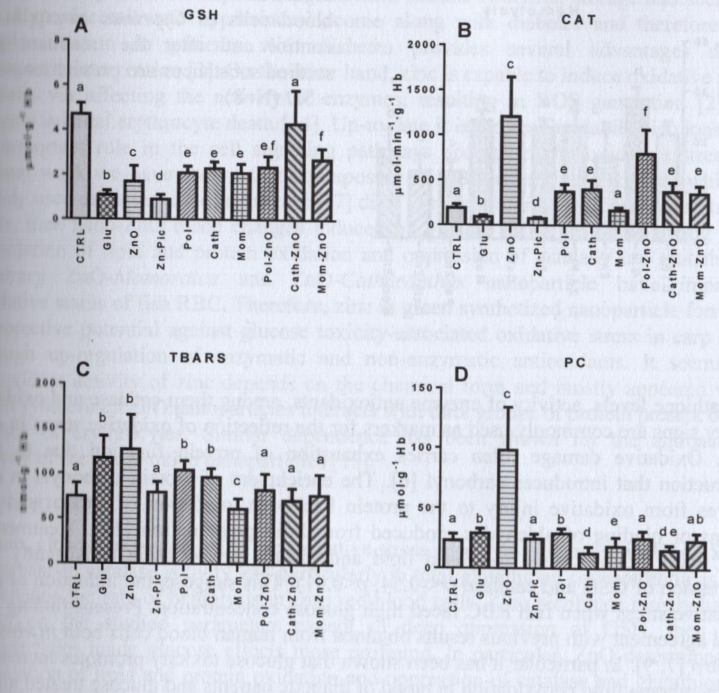

Figure 1. Oxidative stress parameters in the red blood cells of *Cyprinus carpio* in the control and after the exposure to glucose, zinc picolinate, manufactured ZnO nanoparticles, herbal extracts (*Polymnia (Smallanthus) sonchifolia, Catharanthus roseus* and *Momordica charantia)* and green synthetized ZnO nanoparticles are present as means ± SD (N=8). The columns that share the same letters indicate the values that are not significantly different ($P > 0.05$).

The ability of *Polymnia, Catharanthus* and *Momordica* ZnO-containing complexes to protect RBC from glucose-induced cell lysis was first investigated. Extensive hemolysis was induced in the presence of glucose alone (Fig.2) while cells co-exposure with herbal extracts (except of *Polymnia*) and particularly with ZnO-herbal complexes the oxidants demonstrated reduced rate of hemolysis when faced with glucose. Zinc picolinate and ZnO also favoured an increase in stability of RBC.

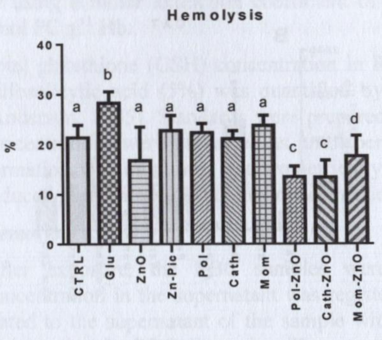

Figure 2. Rate of hemolysis of the red blood cells of *Cyprinus carpio* in the control and after the treatment with studied substances are present as means ± SD (N=8)

Glutathione levels, activity of enzyme antioxidants, among them catalase and oxidative injury signs are commonly used as markers for the reflection of oxidative stress in cells [12]. Oxidative damage often carries exhaustion of protein function due to their destruction that introduces carbonyl [6]. The enrichment of protein carbonyls in cells arrives from oxidative injury to the protein backbone, oxidation of amino acid side chains or binding of aldehydes produced from lipid peroxidation [13]. Treatment of RBC with glucose alone increased lipid and protein peroxidation consistently with oppression of GSH and catalase (r<-0.54, p<0.01). This suggests the induction of deep oxidative stress when fish RBC faced high glucose concentration. Present finding is in good agreement with previous results obtained from human blood cells both *in vivo* and *in vitro* [7, 9]. In particular it has been shown that glucose toxicity promotes increase in the membrane lipid peroxidation in blood of diabetic patients and glucose treated human erythrocytes [7]. High glucose concentration is capable to generate reactive oxygen species from the autooxidation of glucose and glycated proteins with concomitant increase in cellular lipid peroxidation, membrane damage in different cell systems and in diabetic blood [3]. Indeed, carp RBC represent the same response to glucose toxicity like human cells and should serve for deeper understanding of biochemical and molecular *mechanism* implicated early in the development and *progression* of the diabetes.

Co-exposure of RBC with herb extracts namely *M. charantia* and *C. roseus,* but not *P. sonchifolia* protected carp RBC from oxidative stress induced by glucose. In India *M. charantia* is one of the most important plant for lowering blood glucose levels in patients with diabetes [4]. Recently several works have been appeared devoted to exploration of antiglycaemic potentials of *C. roseus,* but mostly in rodent models [5]. Antidiabetic effects of *M. charantia and C. roseus relates to* their ability to improve the performance of pancreatic tissue, which is done by increasing insulin secretions or reducing the intestinal absorption of glucose. Due to our knowledge this is the first attempt where *Catharanthus* extract preserve RBC against oxidative stress. These results have pointed to the necessity of further investigations of antihyperglycemic activity of *Momordica* and *Catharanthus* and mechanistic explanation of their potentials.

Zinc is essential for carbohydrate metabolism, insulin synthesis, storage and secretion [1]. Hypozincemia and hyperzincuria come along with diabetes and therefore zinc supplementation in patients with diabetes provides several advantages during therapeutic intervention [3]. On the other hand, zinc is capable to induce oxidative stress in cells via affecting the activity of enzymes, resulting in ROS generation [2] and triggers suicidal erythrocyte death [14]. Up-to-date it is proven that labile zinc ions play an important role in the cell signaling pathways accompanying oxidative stress. In present work we have shown that co-exposure of RBC with zinc picolinate which is widely used as dietary zinc supplement [7] didn't provoke significant changes in studied traits, then nano-ZnO made changes induced by glucose more profound among them stimulation of lipid and protein oxidation and oppression of catalase and glutathione. Contrary ZnO-*Momordica* and ZnO-*Catharanthus* nanoparticle have improved oxidative status of fish RBC. Therefore, zinc in green synthetized nanoparticle form has a protective potential against glucose toxicity-associated oxidative stress in carp RBC through up-regulation of enzymatic and non-enzymatic antioxidants. It seems the antioxidant activity of zinc depends on the chemical form and mostly appeared when green synthetized ZnO nanoparticles interacts with thiol groups of protein present on the surface of erythrocytes. Similar dependence has been shown for the antibacterial activity of the metal oxide nanoparticles [15].

CONCLUSION

In sum, glucose exposure led to the oxidative stress appeared as increase in TBARS, but a decrease in catalase activity and particularly in total glutathione concentration as well as enhance the rate of hemolysis in carp red blood cells. Zinc picolinate mostly had no effect on the studied parameters except of deep oppression of GSH, then ZnO nanoparticles made glucose effects more profound. In particular, ZnO determined the stimulation of lipid and protein oxidation and oppression of catalase and glutathione in red blood cells of *C. carpio. Momordica* extract, ZnO-*Momordica* and ZnO-*Catharanthus* complexes provoked the most prominent changes related to the decreased in TBARS and rate of hemolysis, and the increased in catalase and glutathione when compared to the glucose treatment alone and brought values in most cases back to control. Obtained results have disclosed the necessity of further studies of antihyperglycemic activity of *M. charantia* and *C. roseus* as well as their green-synthetized ZnO nanoparticle and mechanistic explanation of their potentials.

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COMPUTER SIMULATION OF COMPOSITION COATINGS WITH SET PROPERTIES

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ABSTRACT

The main purpose of this scientific work is to review the current methods of multifunctional material design, and to establish approaches based on multiscale non-deterministic analyzes that can be used to model composite coatings. Analyzing of the literature data showed that methods of computer modeling of materials can be classified by the following. The first group represents approaches in which for selected values of functional properties the process of selecting materials is based on a combinatorial search in the experimental database. The second one is a computer simulation based on computational methods and the theoretical foundations of physical materials science, where a bottom-up approach, including quantum and molecular modeling, is used to accelerate the discovery of new materials. The third is the method of modeling materials, based on the integration of computational stimulation, system engineering, production and design. It is established that all the listed approaches are designed for bulk materials and are not adapted for protective coatings. Therefore, the creation of methods for modeling computer design of composite coatings with given functional properties is an important task in the field of information systems.

Keywords: composition coatings, computer simulation, mathematical model, set properties, calculation methods

INTRODUCTION

The process of selecting protective coatings in the field of materials science was based on the use of tabular data on mechanical, physical and other properties [1]. The modern trend has shifted towards the composition of materials and the connection of the microstructure and properties of the system components. The purpose of the creation of composite coatings with various special, sometimes contradictory, properties [2]. In the past, development of new composite coatings took a lot of time and with a large amount of effort: experimenters obtained protective coatings under various regimes, studied their properties, and out of hundreds of specimens selected the best one [3-7]. Then there was tries to design the technique of development compositions with set properties. This process could take decades and frequently had big material cost. The need of development of technique that could give prediction with no error revealed itself. Meaning that not experimenting in laboratories but give a task to computer to make prediction, which coating with certain composition construction and microstructure will have certain required properties under certain operating conditions [8-10].

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