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CHARACTERIZATION AND PHOTOCATALYTIC INVESTIGATION ON COPPER OXIDE CONTAINING CATALYST

ОХАРАКТЕРИЗИРАНЕ И ФОТОКАТАЛИТИЧНО ИЗСЛЕДВАНЕ НА КАТАЛИЗАТОР СЪДЪРЖАЩ МЕДЕН ОКСИД

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Abstract: New type of photocatalyst containing copper oxide hydrate crystalline phase and additional amount of copper sulfate hydroxide was prepared by thermal decomposition of copper sulfate. The EPR detected presence of Cu^{2+} ions. Photocatalytic degradation of two different model pollutants Reactive Black 5 (RB5) and Malachite Green (MG) in aqueous solution under UV illumination was investigated. The copper oxide containing catalyst showed four times higher photocatalytic activity with respect to RB5 than that to MG dye. The catalyst exhibited much higher adsorption capacity to RB5 than to MG dye. The degree of degradation of MG dye is 18%, rate constant is $1.7 \times 10^{-3} \text{ min}^{-1}$ while the degree of degradation of RB5 dye is 90%, rate constant is $8 \times 10^{-3} \text{ min}^{-1}$ after 2 hours of illumination.

Keywords: COPPER OXIDE, REACTIVE BLACK 5, MALACHITE GREEN, PHOTOCATALYSIS, WASTEWATERS

1. Introduction

CuO is p-type semiconductor with a narrow band gap of 1.21–1.51 eV and monoclinic structure [1]. It is an interesting multifunctional material due to its promising applications in gas sensors [2, 3], magnetic storage media [4], lithium ion batteries [5], and solar cells [6] due to its photoconductive and photochemical properties. In most reports composite photocatalyst for dye degradation such as: CuO/SnO_2 , CuO/ZnO , CuO/BiVO_4 , CuO/SiO_2 , $\text{CuO}/\text{zeolite}$ [7], $\text{CuO}/\text{graphene}$ [8], chitosan anchored copper oxide [9] were used but in recent years also pure CuO was studied [10]. CuO was tested as an adsorbent in the Methylene Blue dye decolorization process [11]. Cu-core/ CuSO_4 -shell nanoparticles exhibited higher photocatalytic efficiency than Cu nanoparticles and these results proved that CuSO_4 -shell has significant effect on the degradation of Methylene Blue [12]. Enormous amounts of environmental pollutants, effluents of colored dyes having carcinogenic effect are discharged by the textile and paper industries [13]. These dye pollutants are chemically stable, so technologies relating to direct UV photolysis and hydrogen peroxide oxidation are not effective in removing the color dyes. At present, the photocatalytic method attracts considerable attention due to its effective decolorization of dyes [14]. Malachite Green (MG) has now become a highly controversial compound due to the risks it poses to the consumers of treated fish, including its effects on the immune system and reproductive system and its genotoxic and carcinogenic properties [15]. The photocatalytic efficiencies of cerium-cadmium oxide [16], $\text{ZnS}-\text{CdS}$ [17], bismuth oxide [18], TiO_2 [15], CuO supported on HY zeolite [19] and other catalysts were tested by using them in the photocatalytic degradation of Malachite Green dye. Sonophotolytic degradation of azo dye Reactive Black 5 (RB5) in an ultrasound/UV/ferric system was examined [20] as well as the efficiency of the $\text{Fe}_3\text{O}_4/\text{FeC}_2\text{O}_4$ magnetic catalyst in the catalytic wet peroxide oxidation of reactive azo dye RB5 [21]. Our previous research has shown high photocatalytic activity of TiO_2 films in the degradation of RB5 dye under UV light [22].

The aim of this article is to characterize by PXRD, XPS and EPR analysis copper oxide containing catalyst synthesized by thermal decomposition of copper sulfate. Because of its recent application in photocatalysis we set ourselves the task to examine its photocatalytic properties in regard to oxidative degradation of two hazardous textile dyes- Reactive Black 5 and Malachite Green.

2. Experimental

2.1. Synthesis of the samples

For preparation of CuO containing sample we used $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$ as starting reagent. The suspension of copper sulfate and water was magnetically stirred upon heating for about 1h. After that the obtained sample was dried at 100°C for 12 h. The finally obtained powder was annealed for 3 h at 500°C in air.

2.2. Powder X-ray diffraction analysis (PXRD)

The PXRD of the obtained photocatalyst was carried out using a TUR M62 apparatus, Germany with PC control and data acquisition, using HZG-4 goniometer and $\text{CoK}\alpha$ radiation. The presence of the phases registered in PXRD pattern was established by using of JCPDS database (Powder Diffraction Files, Joint Committee on Powder Diffraction Standards, Philadelphia PA, USA, 1997).

2.3. Electron paramagnetic resonance (EPR)

The EPR spectrum was recorded on JEOL JES-FA 100 EPR spectrometer operating in the X-band with standard TE011 cylindrical resonator. Spectra were recorded at room temperature.

2.4. X-ray photoelectron spectroscopy (XPS)

The X-ray photoelectron spectroscopy (XPS) studies were performed in a VG Escalab II electron spectrometer using $\text{AlK}\alpha$ radiation with energy of 1486.6 eV under base pressure 10^{-7} Pa and a total instrumental resolution of 1 eV. The binding energies (BE) were determined utilizing the C 1s line (from an adventitious carbon) as a reference with energy of 285.0 eV. The accuracy of measuring the binding energy was 0.2 eV. The O 1s, Cu 2p and S 2p, photoelectron lines were recorded and corrected by subtraction of a Shirley's-type of background and quantified using the peak area and Scofield's photoionization cross-sections.

2.5. Catalytic activity tests

The photocatalytic activities of the prepared samples were measured in oxidative degradation of both Reactive Black 5 (RB5) dye and Malachite Green (MG) under UV light. The photocatalytic

studies were performed using UV-Vis absorbance spectrophotometer in the wavelength range from 200 to 800 nm and a polychromatic UV-A lamp illumination (18W) with maximum emission at 365 nm. The initial concentration of the used RB5 and Malachite Green dye solutions was 20 ppm and 5 ppm respectively. The photocatalytic tests were carried out under slightly acidic pH=6. Before switching on illumination, the catalyst and dye solution were stirred for 30 min in dark to achieve adsorption equilibrium. The degree of degradation of the dyes is calculated using equation (1), where C_0 is the initial concentration (based on absorbance) of the dye, C is the residual concentration of the dye after 120 min of illumination.

$$\text{Degradation}[\%] = \left[\frac{C_0 - C}{C_0} \right] \times 100 \quad (1)$$

3. Results and discussions

Figure 1 represents powder X-ray diffraction spectrum of the obtained copper oxide containing photocatalyst. The PXRD results established the presence of copper oxide hydrate phase ($\text{CuO} \cdot 3\text{H}_2\text{O}$) (PDF-36-0545) and additional amount of copper sulfate hydroxide ($\text{Cu}_3(\text{SO}_4)(\text{OH})_4$) (PDF-76-1621). The incomplete thermal decomposition of the starting material copper sulfate is the possible reason for existence of intermediate precursor phase copper sulfate hydroxide registered in the PXRD pattern of prepared copper oxide containing catalyst.

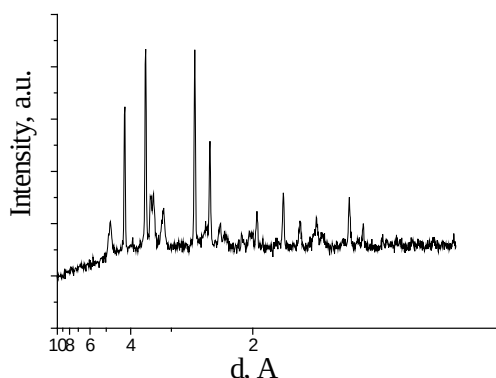


Fig. 1 PXRD pattern of synthesized copper oxide containing photocatalyst.

Figure 2 illustrates the results of electron paramagnetic resonance method. EPR spectrum of CuO containing catalyst at room temperature is consisting of an asymmetric line with g factor 2.24 most probably due to interacting Cu^{2+} ions in clusters [23, 24]. The effect of dipolar interaction between Cu^{2+} ions leads to broadening of individual lines. For this reason the hyperfine structure due to $I=3/2$ of Cu^{2+} ion cannot be seen.

The XPS Cu 2p spectrum of the catalyst sample is shown in Figure 3. The “shake-up” satellite located at 944 eV position and a peak at 935.5 eV are clearly visible. The “shake-up” satellite is an evidence of Cu (II) ions [25], while the peak at 935.5 eV coincides with the known CuSO_4 peak position at 935.4 eV [26]. A low intensity peak at 933.6 eV is typical of the CuO peak [26]. The results indicate incomplete transformation of CuSO_4 into CuO, most probably due to the low temperature of treatment.

Figure 4 represents the course of the photocatalytic reaction as dye concentration decrease with the time of illumination of both investigated model pollutants on the CuO containing photocatalyst. The prepared photocatalyst showed four times higher photocatalytic activity to RB5 than MG dye. It has to be noted that the catalyst exhibited much higher adsorption capacity with respect to RB5 than

to MG for 30 min in dark. The degree of discoloration after 2 hours irradiation for MG is 18%, while for RB5 dye is 90% (Figure 5).

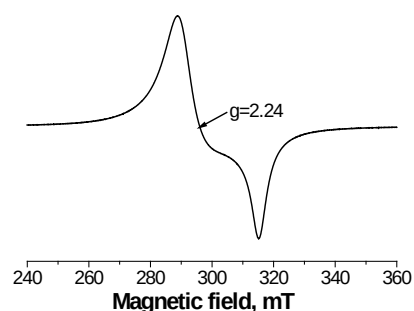


Fig. 2 EPR spectrum of copper oxide containing photocatalyst.

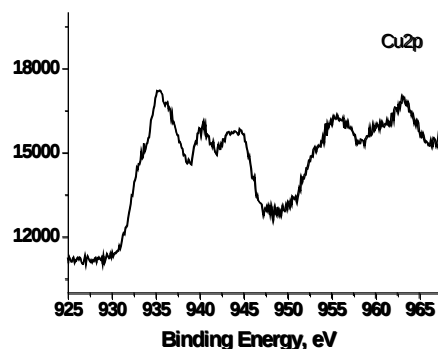


Fig. 3 XPS spectrum of copper oxide containing photocatalyst.

Figure 6 show the dependences of $-\ln(C/C_0)$ as a function of time t under UV light illumination. The dependence shows that the copper containing catalysts exhibit higher photoreactivity to Reactive Black 5 than MG dye in the first 15 minutes of illumination. The photocatalyst has very low activity in degradation of Malachite Green probably due to the difference in the size of conjugated system of C=C and C-C bonds in the molecular structure of the both dyes and different bond scission energies. The rate constants and degree of degradation for the dyes over CuO containing photocatalyst after 120 minutes of UV irradiation are represented in Table 1. The rate constants k after 2 hours for MG and RB5 are $1.7 \times 10^{-3} \text{ min}^{-1}$ and $8 \times 10^{-3} \text{ min}^{-1}$, respectively. Rate constants were calculated using the equation $-\ln(C/C_0) = kt$ on the basis of the slope of the linear logarithmic function.

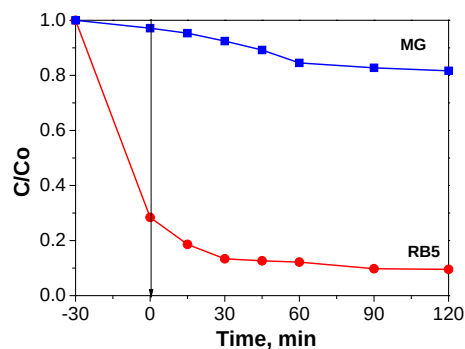


Fig. 4 Concentration changes of both textile dyes based on changes in the intensity of the maximal absorbance peak at 599 nm for RB5 dye and at 615 nm for MG dye respectively, with the course of time.

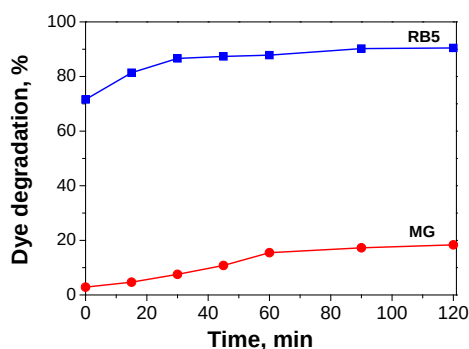


Fig. 5 Degradation degrees of two textile dyes: RB5 and MG over CuO containing powder.

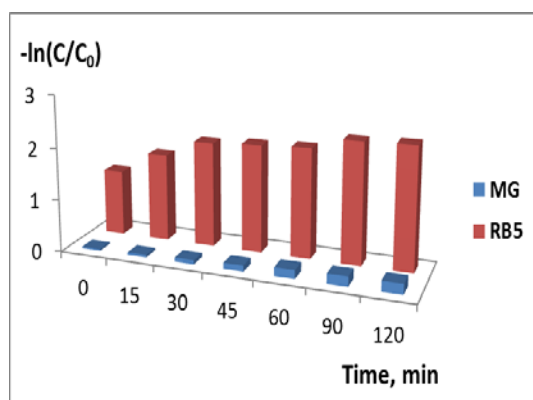


Fig. 6 Dependence of $-\ln(C/C_0)$ with the time of UV illumination for two textile dyes: RB5 and MG over CuO containing photocatalyst.

Table 1. Rate constants and degree of degradation for the both dyes over CuO containing photocatalyst.

Model dye	Rate constant, k ($\times 10^{-3} \text{ min}^{-1}$)	Degradation, % after 120 min
MG	1.7	18
RB-5	8	90

The adsorption spectrum of RB5 has two adsorption peaks corresponding to the $\text{N}=\text{N}$ - bond (at 599 nm) and to naphthalene rings (at 313 nm). Oxidative attack of an azo dye from the phenyl azonaphthol family as RB5 leads to the formation of benzene derivatives and naphthoquinone as primary degradation products. The scheme of possible degradation of Reactive Black 5 can be seen in [22].

The higher photocatalytic efficiency of copper containing photocatalyst to oxidize the azo dye RB5 than those to MG the double ($\text{N}=\text{N}$ -) bond in RB5 is weakened by hyperconjugation and N,N -dimethylaminobenzyl in MG [27]. However the central carbon atom possesses also a double bond, connecting it to the third cyclohexadiene ring, which requires also high energy photon for the bond scission. The C-C bond between the central carbon atom and N,N -dimethylaminobenzyl in MG, results in the formation of 4-(N,N -dimethylamino) methylbenzylone as most common intermediate [28,29]. The decisive argument explaining the activities is the difference in the size of the two conjugated systems. According to the results for Cu-core/ CuSO_4 -shell nanoparticles possess higher photocatalytic efficiency than Cu nanoparticles [12].

In our case probably the same effect of the presence of copper sulphate plays positive role in the photocatalytic degradation. The results obtained in this article for copper containing photocatalysts are in accordance with our previous studies on ZnO films [29].

4. Conclusions

Photocatalyst containing hydrated copper oxide crystalline phase and additional amount of copper sulfate hydroxide was prepared by thermal decomposition of copper sulfate. The performed PXRD and XPS studies confirmed the presence of copper oxide and some quantity of copper sulfate hydroxide phases. The EPR analysis detected the existence of Cu^{2+} ions in obtained material. The copper oxide containing photocatalyst showed strong difference in its photocatalytic behaviour with respect to the two model dyes, due to differences in their structure and physicochemical properties. The photocatalyst possess much higher adsorption capacity and selectivity to degrade the double diazo bond in RB5 in comparison to the two single carbon-carbon bond in MG. We can recommend copper oxide containing material as relatively new cheap alternative to the already used photocatalysts for degradation of textile azo dyes.

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EFFECT OF La DOPING AND THERMAL TREATMENT ON THE PHOTOCATALYTIC ACTIVITY OF ZnO FOR DEGRADATION OF REACTIVE BLACK 5 DYE

ВЛИЯНИЕ НА La-ДОТИРАНЕТО И ТЕРМИЧНАТА ОБРАБОТКА ВЪРХУ ФОТОКАТАЛИТИЧНАТА АКТИВНОСТ НА ZnO ЗА РАЗГРАЖДАНЕ НА РЕАКТИВНО ЧЕРНО 5 БАГРИЛО

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Abstract: The La-doped powder-form ZnO samples were prepared by impregnation using appropriate amounts of aqueous solutions of $\text{La}(\text{NO}_3)_3$. The non-impregnated and impregnated zinc oxide materials were then thermally treated at different temperatures – 350°C and 450°C in air atmosphere. The phase composition and structure of the obtained catalysts were characterized by powder X-ray diffraction analysis (PXRD), EPR and X-ray photoelectron spectroscopy. The PXRD results gave evidence that the average crystallite size of nanosized ZnO phase was varying within the range of 10-14 nm. The present work was focused on the influence of La doping and calcination temperatures on the photocatalytic activities of zinc oxide samples in the reaction of oxidative degradation of industrial textile azo dye Reactive Black 5 (RB5) under UV-light irradiation. The photocatalytic activity tests showed that the La doped ZnO photocatalysts are superior to the non-doped samples and are applicable to decontamination of the textile waste waters.

Keywords: REACTIVE BLACK 5 DYE, La DOPED ZnO, PHOTOCATALYST, PHOTOCATALYTIC ACTIVITY

1. Introduction

Organic dyes find various applications, such as industrial chemicals (textile dyes, surfactants), pharmaceuticals (antibiotics, steroids), antifouling compounds, histopathological applications and staining agents in bacteriological studies. Lately the attention is directed to the elimination or mineralization of different persistent organic pollutants [1].

Wide band-gap semiconductors, such as TiO_2 , ZnO are the promising materials in water purification and disinfection, air purification and hazardous waste neutralization. The photocatalytic efficiency of these oxides in the degradation of different environmental contaminants attracts attention recently [2].

It has been evidenced that the properties of ZnO can be significantly improved by doping with rare-earth elements, which have specific appropriate electronic structure [3]. Lanthanide (Ln = La, Eu, Gd, Dy and Ho) loaded ZnO catalysts (Ln-ZnO) were prepared, characterized and investigated for the discoloration of Methyl Orange [4]. Tingting Wu and coworkers established that La-doped ZnO nanoparticles, obtained by a simple solution combustion method, have superior capacities for the removal of Pb^{2+} and Cu^{2+} ions in waterways than the undoped ZnO nanoparticles [5]. Optical and photocatalytic properties of La-doped ZnO nanoparticles synthesized via precipitation and mechanical milling method are discussed in [6]. The investigations proved that the photocatalytic efficiency in degradation of a Methylene Blue solution using these samples depended upon the number of oxygen vacancies [6]. La-doped ZnO nanowires with different dopant contents were obtained via a solvothermal synthesis route, using ethanol as the solvent. The photocatalytic activity of pure ZnO and La^{3+} -doped ZnO samples was investigated in the degradation of Rhodamine B. The results established that 2 at% of La^{3+} -dopant content in ZnO attribute enhanced photocatalytic efficiency [7].

The present study deals with the effect of La doping and thermal treatment on the photocatalytic properties of zinc oxide materials. For this purpose the synthesis of La doped ZnO samples using impregnation method and calcination at different temperatures were applied. The photocatalytic activity of prepared non-impregnated and impregnated zinc oxide samples was tested

and compared in the reaction of oxidative degradation of Reactive Black 5 dye (RB5) under UV-light irradiation.

2. Experimental

2.1. Preparation of photocatalysts

The method of preparation of activated ZnO powder was described in a Bulgarian Patent [8]. The preparation procedure includes dissolution of commercial ZnO in NH_4OH solution, followed by precipitation as $\text{Zn}(\text{OH})\text{CO}_3$ as a result of CO_2 bubbling through the solution. The La-doped ZnO samples were prepared by impregnation of $\text{Zn}(\text{OH})\text{CO}_3$ with aqueous solution of $\text{La}(\text{NO}_3)_3$ to obtain 1.5wt % La content in La/ZnO composite. The non-impregnated and impregnated zinc oxide materials were then thermally treated at different temperatures – 350°C and 450°C - for 2 hours in air atmosphere. The so prepared samples were denoted as: ZnO-350°C, ZnO-450°C, La/ZnO-350°C and La/ZnO-450°C.

2.2. Methods for investigations of obtained samples

The powder X-ray diffraction patterns (PXRD) of the synthesized powders were recorded on a TUR M62 apparatus, Germany with PC control and data acquisition, using HZG-4 goniometer and $\text{CoK}\alpha$ radiation. The identification of the phases registered in PXRD patterns was accomplished based on JCPDS database (Powder Diffraction Files, Joint Committee on Powder Diffraction Standards, Philadelphia PA, USA, 1997).

The EPR spectra were recorded on JEOL JES-FA 100 EPR spectrometer operating in the X-band with standard TE011 cylindrical resonator. The sample was placed in a special EPR tube and it was positioned in the center of the EPR cavity. All measurements were made in air at room temperature.

The X-ray photoelectron spectroscopy (XPS) studies were performed in a VG Escalab II electron spectrometer using $\text{AlK}\alpha$ radiation with energy of 1486.6 eV under base pressure of 10^{-7} Pa and a total instrumental resolution 1eV. The binding energies (BE) were determined utilizing the C 1s line (from an adventitious

carbon) as a reference signal of energy of 285.0 eV. The accuracy of the measured binding energy was 0.2 eV. The O 1s, Zn 2p, La 3d_{5/2}, photoelectron lines were recorded and corrected by subtraction of a Shirley's type of background and quantified using the peak area and Scofield's photoionization cross-sections.

2.3. Photocatalytic study

The photocatalytic oxidative degradation of Reactive Black 5 (RB5) was carried out using 150 ml dye aqueous solution with initial concentration of 20 ppm. Photocatalytic activity measurements were accomplished using polychromatic UV-A lamp illumination (18 W, 320-400nm) with a maximum of the emission at 365 nm. The process of discoloration was monitored by UV-Vis spectrophotometer CamSpec M501, based on the absorbance of the dye solution in the wavelength range from 200 to 800 nm. The samples were equilibrated in the dark for about 30 min before switching on the illumination. In order to study the photocatalytic activity of ZnO and La-doped ZnO materials, sample aliquots of the suspension were taken away from the reaction vessel at regular time intervals and filtered. The rate constant k was determined as the slope of the linear dependence on time t : $-\ln(C/C_0) = kt$ (where C_0 and C are initial concentration before switching on the irradiation and residual concentration of the solution after illumination for the chosen time interval at 599 nm absorbance maximum, attributed to the peak of the diazo bond (-N=N-)).

3. Results and discussion

The PXRD patterns of prepared non-impregnated ZnO and impregnated La/ZnO samples thermally treated at 350°C and 450°C are represented in Figures 1-4. The presence of ZnO phase (PDF-36-1451) is determined in recorded PXRD spectra of all obtained samples. No La-containing phases could be registered probably because of the low content of La in the La doped ZnO photocatalysts. The calculations of average crystallite size by using PowderCell for Windows Version 2.4 software [9] show that the prepared ZnO and La-doped ZnO materials are nanosized with mean crystallite size of about 10-14 nm.

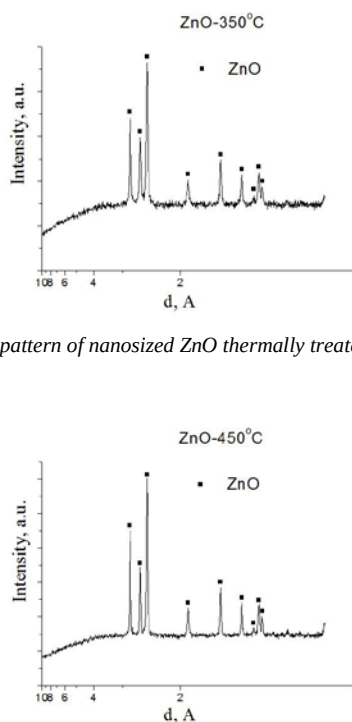


Fig. 1 PXRD pattern of nanosized ZnO thermally treated at 350°C.

Fig. 2 PXRD pattern of nanosized ZnO thermally treated at 450°C.

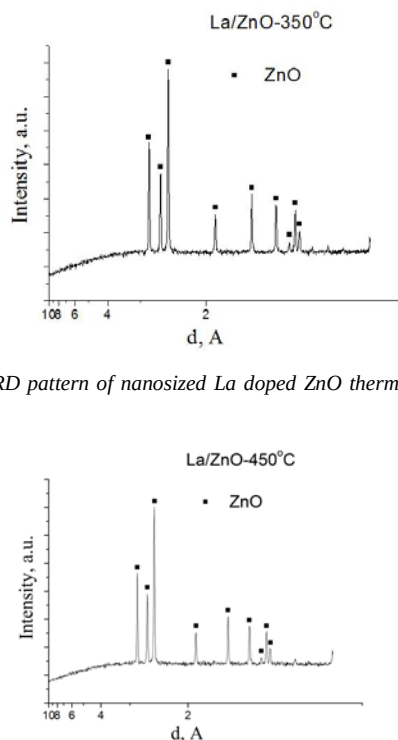


Fig. 3 PXRD pattern of nanosized La doped ZnO thermally treated at 350°C.

Fig. 4 PXRD pattern of nanosized La doped ZnO thermally treated at 450°C.

Electron paramagnetic resonance is a powerful tool to monitor the paramagnetic charge states of vacancies/defects in ZnO. Figure 5a shows the EPR spectrum of ZnO nanocrystals at room temperature, which shows the resonance signal at $g=2.0784$. This signal was attributed to a shell, whose core contains high concentration of surface defects [10]. Such defects have been identified as negatively charged Zn vacancies acting as shallow acceptors [11,12]. When ZnO nanoparticles are modified with La, their EPR spectrum is changed. The spectrum is shown in Fig. 5b. It is interesting to observe that, upon modification of ZnO with La the number of Zn vacancies is decreased. This fact is evidenced by decrease in the resonance signal at $g=2.0784$. In addition a single EPR signal at the g value of 1.9749 has appeared. This signal is attributed to positively charged oxygen vacancies acting as deep donors [12]. Therefore the superior photocatalytic activity of La/ZnO catalyst for oxidative degradation of RB5 dye is probably due to the oxygen vacancies formed during deposition of La on the ZnO surface.

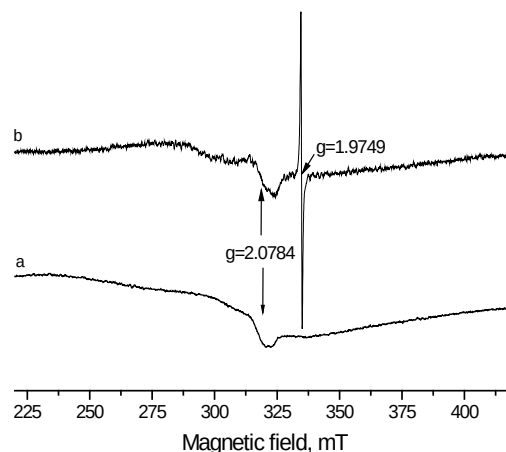


Fig. 5 EPR spectrum at room temperature of: a) ZnO; b) La/ZnO thermally treated at 450°C.

As it has already been discussed in our previous investigation [13] on ZnO and doped ZnO catalysts the surface hydroxyl groups play important role in the mechanism of photocatalytic oxidation.

The investigated O1s photoelectron spectra are represented in Figure 6. It is obvious that there is presence of some more oxygen groups (in addition to the lattice O^{2-}) in both types of ZnO catalysts as well as in the La doped ZnO thermally treated at 350°C and 450°C. The thermal treatment at 450°C leads to appearance of more defects in the both pure ZnO and La-doped ZnO. The higher binding energy shoulder at around 531.5 eV in the O1s photoelectron spectra supplies evidence for that. The percentage of this type of oxygen in the total amount of oxygen, evaluated after deconvolution of the obtained spectra, is increasing from 26.4% up to 35.2% for the ZnO (350°C) and ZnO (450°C), respectively. The same tendency is observed for the La doped ZnO catalyst thermally treated at either of the two temperatures. The percentage of the oxygen, associated with defects, changes with the temperature increase from 24.3% for La/ZnO (350°C) to 35.5 % for La/ZnO (450°C) catalysts. It is worth mentioning here that the formation of additional surface sites in the La-doped ZnO treated at 450°C was detected, which we attributed to water adsorption. The $La_{3d_{5/2}}$ photoelectron peaks of both La-doped ZnO catalysts have been subjected to deconvolutions process, too. The multiplet splitting is typical of the $La(OH)_3$ [14,15], which explains the existence of the additional surface states detected over La/ZnO (450°C).

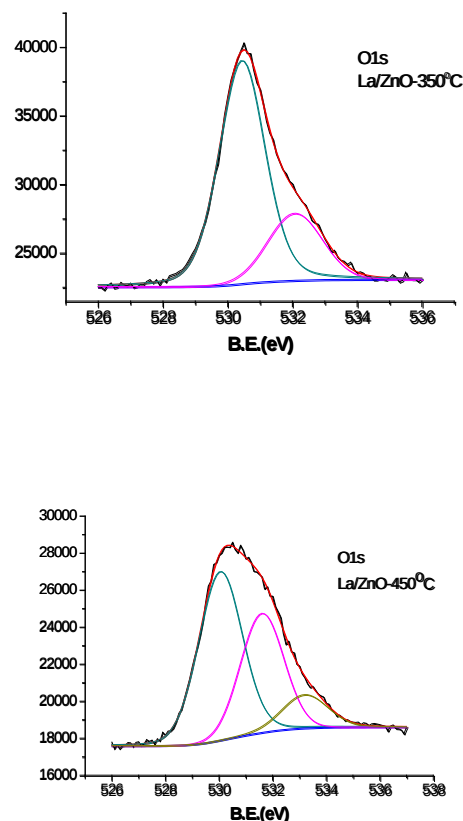
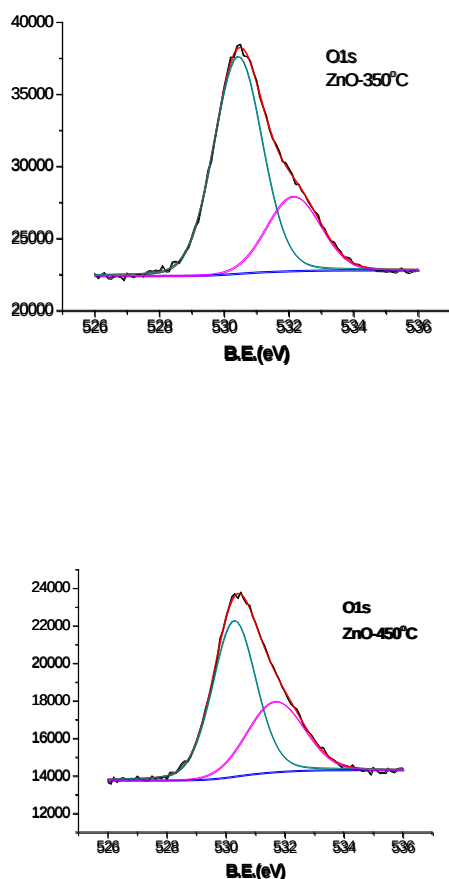


Fig. 6 XPS spectra of nanosized ZnO thermally treated at 350 °C; 450°C and La doped ZnO at 350°C; 450°C.

The photocatalytic activity tests showed that the higher degree of degradation of RB5 dye was achieved in the case of La doped ZnO in comparison with non-impregnated ZnO catalysts. The doping with La influences both the adsorption capacity and photocatalytic efficiency of the samples. As it can be seen from Figures 7 and 8 the doped samples adsorb more dye than the non doped photocatalysts. A. Neren Ökte also reported that La dopant in ZnO promotes higher adsorption capacity and the reaction rate constant values for degradation of the azo dye (Methyl Orange), which is in accordance with our results [4]. The calculated rate constants of prepared nanosized La doped ZnO and ZnO materials thermally treated at 350°C and 450°C approximating to first order kinetics decreases in the following order $La/ZnO-350^{\circ}C$ ($30.4 \times 10^{-3} \text{ min}^{-1}$) > $La/ZnO-450^{\circ}C$ ($30.1 \times 10^{-3} \text{ min}^{-1}$) > $ZnO-450^{\circ}C$ ($14.7 \times 10^{-3} \text{ min}^{-1}$) > $ZnO-350^{\circ}C$ ($6.8 \times 10^{-3} \text{ min}^{-1}$). The rate of oxidative degradation reaction is also higher in the case of lanthanum doped powders. Another research group has also proved the positive effect of La on the photocatalytic degradation rate of the dyes [16].

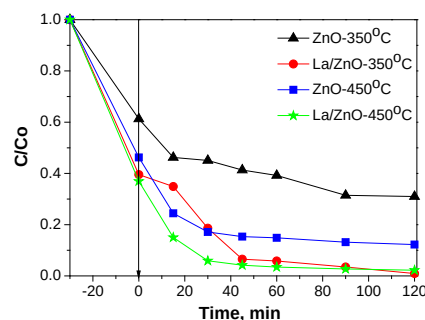


Fig. 7 Reaction course as concentration ratio varying during the photocatalytic oxidation of an initial concentration (C_0) of 20 ppm RB5 dye, based on changes in the intensity of the absorbance peak, corresponding to azo bond ($-N=N-$) as a function of the time interval of irradiation.

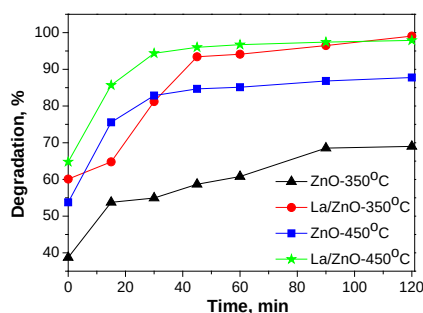


Fig. 8 Degradation of the RB5 dye solution (as conversion degree) after 120 minutes of UV-A illumination over nanodimensional ZnO and La doped ZnO samples calcined at 350°C and 450°C.

It is well known that the photocatalytic activity is closely related to the concentration of defects on the surface of the nanomaterials. The positive effect of lanthanum doping can be explained by the formation of charged surface region due to the surface donor defects on ZnO. The presence of such a region leads to hindered recombination of electrons and holes pairs in ZnO thereby enhancing the photocatalytic efficiency [1,17]. This enhancement of photocatalytic activity of La-doped ZnO can also be explained by more efficient charge carrier separation [18].

We have also studied the influence of calcination temperature on the phase composition, structure and photocatalytic efficiency of doped and non-doped samples. The non-doped powders treated at higher calcination temperature exhibit higher activity than the samples, treated at lower (350°C) temperature. This effect could be due to the higher degree of crystallinity of the samples treated at 450°C (Figure 2). The effect of calcination temperature is less pronounced in the case of doped samples: 99% vs 98% degradation for thermally treated at 350°C and 450°C La/ZnO powders.

4. Conclusions

The present photocatalytic research work established that the degree of degradation of RB5 dye using La doped ZnO is higher than that in the case of non-impregnated ZnO photocatalysts. The higher calcination temperature - 450°C for non-impregnated ZnO leads to increase in the degree of degradation of RB5 (88%), which is superior to that of the ZnO sample calcined at 350°C (69%). The calcination temperature has only a slight effect on the degradation rate over La doped ZnO photocatalysts: 99% vs 98% degradation degree for those thermally treated at 350°C and 450°C, respectively. The La doping of non impregnated ZnO samples leads to increasing of their photocatalytic activity in the reaction of oxidative degradation of RB5 dye used as model contaminant.

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THE METHOD OF GNSS POSITIONING AVAILABILITY CONTROL FOR TRANSPORTATION APPLICATIONS

МЕТОД КОНТРОЛЯ ДОСТУПНОСТИ НАВИГАЦИОННЫХ ОПРЕДЕЛЕНИЙ GNSS ДЛЯ ТРАНСПОРТНЫХ ПРИЛОЖЕНИЙ

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Abstract: A new method of real-time GNSS user positioning availability control for transportation applications is considered. The positioning availability value is defined as a full probability of event when we get a personal GNSS user's required navigation parameters (RNP) taking in account the current Positioning Delusion of Precision (PDOP), ranging errors and positioning errors. On a basis of GNSS/LAAS network dataset we get current GNSS performance statistics, such as positioning error standard mean and standard deviation and a number of positioning failures within the observation period. The PDOP values are used in order to compute an alarm index of a probable sudden positioning deterioration under poor GNSS satellite vehicles (SV) geometry. The method can be recommended for some transportation applications which have strong RNP. Especially, the method can be recommended for transportation applications such as aviation landing systems and automatic railroad traffic control.

KEYWORDS: GNSS/GBAS AVAILABILITY CONTROL; GNSS, GPS, GLONASS, LAAS PERFORMANCE; GNSS TRAFFIC CONTROL

1. Introduction

High positioning accuracy and positioning reliability of GNSS users can be achieved by means of ground-based augmentation systems (LAAS or WAAS). Combining augmentation systems with receiver autonomous integrity monitoring algorithms (RAIM) we can get the efficient solutions for real-time positioning quality monitoring. It allows warning GNSS users about dangerous positioning quality deterioration in time [1]. Combining GNSS and LAAS (or WAAS) we get the most effective mean to achieve high accuracy and quality of transportation automatic control.

Unfortunately both GNSS and LAAS (WAAS) performance is affected by irregular external disturbances such as Space Weather events, multi-path effects and electromagnetic jammers. So, it is well known that geomagnetic storms can cause the signal tracking loss inside the GNSS receivers as well as sharp increasing of ranging errors [2,3]. The other negative Space Weather factor for GNSS and LAAS (WAAS) performance is the powerful solar radio flares in 1-2 GHz frequency band. As it was shown in [4,5], a numerous short-time failures of GPS and GLONASS SV ranging were observed during the powerful solar radio flares on December 6th and 13th, 2006 at some IGS-stations within the Earth sunlit side. Such events can cause serious performance deterioration for both standalone GNSS and LAAS (WAAS) operating [7]. The character of GNSS positioning deterioration varies significantly in space and time under above mentioned conditions. On the other hand, each GNSS user has a personal RNP that can be constant or can change in time (track motto along a railroad or aircraft landing motto, for example). We should say that there are no effective methods of positioning availability control which take in account both irregular external events and personal RNP. However such modern methods are extremely needed in order to provide safety on transportation applications.

We offer a new method of real-time GNSS+LAAS user positioning availability control for transportation applications. The positioning availability value is defined as a full probability of event when we get a personal GNSS user's RNP taking in account the current PDOP, ranging errors and positioning errors. This method can be adopted for aircraft landing applications and for railroad traffic control.

2. The main algorithm for positioning availability control

We consider a case of positioning for GNSS user within the LAAS coverage zone. In order to compute the current positioning availability we use positioning and ranging errors statistics (standard mean and standard deviation), amount of positioning failures and PDOP values which are accumulated and processed at

the LAAS master station within a certain period of time. This time period should not be longer than the positioning errors de-correlation time. According to [7] this time period can be about 30 sec (for the positioning error correlation of 0.7). Being setting personal RNP, each GNSS+LAAS user gets the current positioning availability value from the personal GNSS receiver. The value of positioning availability is computing inside the GNSS receiver on a basis of the data set which is translated from the LAAS master station within the LAAS coverage zone.

The current positioning quality is generally determined by the positioning accuracy and positioning continuity. It is also necessary to detect the "potential positioning failure" which can be caused by the sudden PDOP increasing. Positioning accuracy, continuity and PDOP rapid changing under irregular external influence have all random character in space and time. That is why the positioning availability should be determined in terms of the total probability of the personal RNP availability within LAAS coverage zone. So generally we get the common equation of the positioning availability as following

$$W = P(A) \cdot P(B) \cdot P(C|A, B) \cdot (1 - P_{FAULT}) \cdot W_{PDOP} \quad (1)$$

where A is the event of that GNSS and LAAS equipment are in working order; B is the event of GNSS user equipment health; C is the event that the positioning accuracy corresponds to the personal RNP of GNSS+LAAS user during the certain period of time; $(1 - P_{FAULT})$ is the probability of the absence of positioning failure during the certain period of time; W_{PDOP} – alarm index in order to warn the GNSS user about the dangerous level of expected positioning error as a result of the PDOP value sudden increasing.

In our further consideration we suppose that both GNSS+LAAS and GNSS user equipment have both high reliability, so we get $P(A) = P(B) = 1$.

In order to estimate $(1 - P_{FAULT})$ term, we consider the probable positioning failures as a faults flow. The probability of k number of positioning faults during the certain interval of time (ΔT) can be found through the Poisson law as follows [8]:

$$P_{FAULT} = \frac{a^k}{k!} \cdot \exp(-a) \quad (2)$$

where $k = 0, 1, 2, \dots, n$ is the possible number of positioning faults within the observation period $-\Delta T$, a is the parameter of the Poisson distribution.

The distribution parameter a in (2) depends on the ΔT interval

duration, and the time distribution of positioning faults can be nonstationary within the ΔT period. So the appropriate expedient for the Poisson law parameter a computation is to smooth the histogram of positioning fault events (P_k) by a theoretical curve of Poisson probability (2) for the time interval ΔT using the least-squares method as follows

$$\sum_{k=0}^n \left(P_k - \frac{a^k}{k!} e^{-a} \right)^2 \rightarrow \min \quad (3)$$

where n is the maximum number of positioning faults in a series of observations.

Depending on the area of application there are some features of the parameters $P(C|A,B)$ and W_{PDOP} representation and computation. We considered two probable area of the method application: aircraft landing applications and railroad automatic traffic control.

2.1. Aircraft landing application

Being landing the aircraft should be fixed within the narrow air echelons of ΔX , ΔY , and ΔZ in plane and altitude. According to ICAO requirements the aircraft should be keeping within these echelons with positioning accuracy better than 3 meters at probability of 0.999 or higher. We determine $P(C|A,B)$ term in (1) as follows [9]

$$P(C|A,B) = P_{TX} P_{TY} P_{TZ} \quad (4)$$

The right-hand side of this equation contains probabilities of compliance with the air echelons along the planar and altitudinal axes that can be computed as following [9]

$$P_{TX} \{ \alpha_x < \Delta X_i < \beta_x \} = 0.5 \left[\Phi \left(\frac{\beta_x - M(\Delta X)}{\sigma_x} \right) - \Phi \left(\frac{\alpha_x - M(\Delta X)}{\sigma_x} \right) \right] \quad (5)$$

$$P_{TY} \{ \alpha_y < \Delta Y_i < \beta_y \} = 0.5 \left[\Phi \left(\frac{\beta_y - M(\Delta Y)}{\sigma_y} \right) - \Phi \left(\frac{\alpha_y - M(\Delta Y)}{\sigma_y} \right) \right]$$

$$P_{TZ} \{ \alpha_z < \Delta Z_i < \beta_z \} = 0.5 \left[\Phi \left(\frac{\beta_z - M(\Delta Z)}{\sigma_z} \right) - \Phi \left(\frac{\alpha_z - M(\Delta Z)}{\sigma_z} \right) \right]$$

where $\Phi(\dots)$ is Laplace's function; $M(\Delta X)$, $M(\Delta Y)$, $M(\Delta Z)$, $\sigma_{\Delta X}$, $\sigma_{\Delta Y}$, $\sigma_{\Delta Z}$ – are the standard mean and standard deviation of positioning errors; α and β are admissible minimum and maximum bounds of positioning errors along the X , Y and Z axes (norms of the air echelons according to the ICAO RNP).

The last item - W_{PDOP} in (1) should be specified more clearly. It is known that aircraft positioning accuracy requirements in plane and altitude differs one from another [10]. Thus, the horizontal and vertical delusion of precision factors (HDOP and VDOP) should be considered separately in order to warn airborne user about "potential positioning fault" in horizontal or vertical planes. Finally we can compute the current alarm index W_{PDOP} as follows

$$W_{PDOP} = \begin{cases} 1, & (HDOP \leq \Pi_{HDOP}) \wedge (VDOP \leq \Pi_{VDOP}) \\ 0, & (HDOP > \Pi_{HDOP}) \vee (VDOP > \Pi_{VDOP}) \end{cases} \quad (6)$$

This warning is realized on a basis of personal HDOP and VDOP threshold levels Π_{VDOP} and Π_{HDOP} , which can be found as

$$\Pi_{HDOP} \leq \frac{\left(\sqrt{\sigma_x^2 + \sigma_y^2} \right)_{\max}}{\sigma_{\Delta R}} \quad (7)$$

$$\Pi_{VDOP} \leq \frac{(\sigma_z)_{\max}}{\sigma_{\Delta R}}$$

Where subscript "max" designates the corresponding maximum standard deviations of positioning errors in the plane and in

altitude according to the personal RNP; $\sigma_{\Delta R}$ – standard deviation of ranging errors, which is computed on a basis of ranging of all SV in view on the LAAS master station during the observation period - ΔT .

2.2. Railroad automatic traffic control

The features of this application for our method are following:

1) A train moves along a stringent and well known trajectory, so we do not need to take in account planar and altitudinal positioning deviations, but we need to determine an expected error of the current length of the train braking action way, instead;

2) We do not need to warn user about sudden positioning accuracy deterioration in the vertical plane, so the alarm index - W_{PDOP} can be simplified: only threshold value Π_{HDOP} is enough to compute the current value of W_{PDOP} .

In order to adopt the $P(C|A,B)$ term to the railroad application we should describe some parameters which are critical in process of safe train braking action (look at Fig. 1).

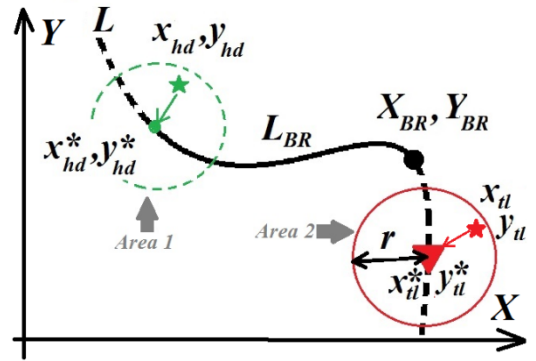


Fig.1. A train collision warning system elements

First we should know the exact position of the railroad trajectory (L) in a special railroad coordinate system (X, Y). Being knowing L coordinates one can compute the current braking action way

(L_{BR}) between (x_{hd}, y_{hd}) and (X_{BR}, Y_{BR}) points on a basis of a special normative "speed instead braking way" curves taking in account the train speed and mass. The coordinates of both train head (x_{hd}, y_{hd}) and forwarding train's tail (x_{tl}, y_{tl}) are got from the GNSS measurements. These coordinates contain positioning errors which are scattered within Area 1 and Area 2, correspondently. In order to compute L_{BR} length we transform the current train head coordinates (x_{hd}, y_{hd}) to the nearest point on the

railroad trajectory (x_{hd}^*, y_{hd}^*) . Being knowing the L_{BR} length and railroad trajectory coordinates we find the finish point of the braking way (X_{BR}, Y_{BR}) on the railroad trajectory.

We have to alarm a train driver about possible train collision if the point (X_{BR}, Y_{BR}) hits inside the Area 2. The center of this area corresponds to a point (X_{tl}^*, Y_{tl}^*) which are found like the above

mentioned (x_{hd}^*, y_{hd}^*) . The radius of the Area 2 depends on the probability of collision which we set. If, say, we established the probability of collision equals to $(1-0.997=0.003)$, then $r \approx 3 \cdot \sigma_r$, where σ_r is equivalent standard deviation of the positioning errors, which is determined as $\sigma_r^2 = \max\{\sigma_{\Delta X}^2, \sigma_{\Delta Y}^2\}$. Finally we determine the $P(C|A,B)$ term as a probability of event when the point (X_{BR}, Y_{BR}) hits inside the Area 2 [8]

$$P(C|A, B) = \exp \left(-0.5 \cdot \left[\frac{(X_{BR} - m_X)^2}{\sigma_X^2} + \frac{\left(Y_{BR} - m_Y - c \cdot \frac{\sigma_Y}{\sigma_X} (X_{BR} - m_X) \right)^2}{\sigma_Y^2 (1 - c^2)} \right] \right) \quad (8)$$

Where c is a correlation coefficient between ΔX and ΔY time series of positioning errors; $m_X = x_{tl}^*, m_Y = y_{tl}^*$ are standard means of positioning errors; σ_X, σ_Y - are standard deviations of positioning errors.

The current alarm index W_{PDOP} for the railroad applications should take in account the horizontal DOP variations only, so we can write

$$W_{PDOP} = \begin{cases} 1, & (HDOP \leq \Pi_{HDOP}) \\ 0, & (HDOP > \Pi_{HDOP}) \end{cases} \quad (9)$$

Where Π_{HDOP} is computed on a basis of equation (7), as above mentioned.

2.3. The algorithm of practical implementation

In order to realize the above mentioned technique continuous monitoring of GPS (GLONASS) SV ranging and positioning errors should be arranged on a ground based LAAS station. These measurements are periodically accumulated within time periods ΔT at LAAS master station so we periodically get time series of the ranging errors $\Delta \mathbf{R} = [\Delta r_1, \Delta r_2, \dots, \Delta r_n]$ and positioning errors

$\Delta \mathbf{\Pi} = [\Delta x, \Delta y, \Delta z]$. On a basis of this data set the master station

PC gets following statistics:

- The frequency histogram of positioning fault events (P_k) over the observation interval ΔT and the parameter a of the Poisson distribution (equations 2 and 3);
 - Current standard means and standard deviations of positioning errors: $M(\Delta X), M(\Delta Y), M(\Delta Z), \sigma_{\Delta X}, \sigma_{\Delta Y}, \sigma_{\Delta Z}$ which are supposed to be the constant within the LAAS coverage zone during the period of ΔT ;
 - Current standard deviation of GPS (GLONASS) SVs ranging ($\sigma_{\Delta RSV}$) for all SVs in view which is supposed to be the constant within the LAAS coverage zone during the period of ΔT .
- User equipment should contain the special software in order to compute the current positioning availability (W , equation 1), getting all the above mentioned statistics from the LAAS master station, as follows:
- Setting the individual positioning accuracy requirement such as α and β boundaries (equation 5) or positioning error probability (equation 8) and maximal standard deviations $(\sigma_X^2 + \sigma_Y^2)_{\max}$ and $(\sigma_Z)_{\max}$ (equations 7);
 - Setting the individual admissible number of positioning faults (k) over ΔT time interval (equations 2 and 3);
 - Computing $P(C/A, B)$ value on a basis of equations (4) and (5) or (8) depending on the application;
 - Computing $(1 - P_{FAULT})$ value (equation 2);
 - Computing Π_{VDOP} and Π_{HDOP} (equation 7);
 - Computing the current positioning availability (W) from equation (1).

As one can see, such method allows detecting sudden positioning quality deterioration for the concrete RNP of aviation or railroad users and can be effectively used for these transportation applications.

Conclusion

As we can see the method of positioning availability control is based on the near-real-time measurements of positioning and ranging statistics, so we can expect an adequate result of availability control within LAAS coverage zone. On the other hand the technique we considered allows taking in account the personal RNP of each user within LAAS coverage zone. This feature of the method is especially important for aircraft landing application. It is well known that personal RNP is changing during the landing process from ICAO CAT I down to ICAO CAT III RNP. Such RNP evolution in time requires a flexible technique of the positioning availability control in near-real time scale.

Being taking in account an individual PDOP factor we can warn user about some local features of the coverage zone. This is especially important for the railroad applications when the user often faces to a problem of SVs ranging faults because of the railroad infrastructure objects influence.

Finally, it is well known, that geomagnetic storms and L-band solar radio flares affect GNSS and Ground based augmentation systems performance significantly. The LAAS (or WAAS) coverage zone size can cut down under unfavorable geophysical conditions. The decorrelation time of ranging and positioning errors can decrease under geomagnetic storms influence too. GNSS satellite signal tracking process often breaks as a result of SVs signal ionospheric scintillations under geomagnetic storms.

All this effects often works concurrently so GNSS performance have to be controlled not only in the near-real time scale but also taking in account personal RNP within LAAS coverage zone. The considered method is appropriate to get an adequate GNSS positioning performance assessment for some transport applications under such complex conditions.

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PLASTIC RESOURCE OF LOW-CARBON STEEL DURING IN TECHNOLOGICAL PROCESS OF DEEP DRAWING

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Abstract: The present study deals with the development of a method involving physical experiment and numerical simulation. The aim is to predict the possibility of maximal use of the plastic resource of a low-carbon steel circular blank subjected to deep drawing. The material hardening curve under uniaxial tension was found experimentally. A series of real physical experiments of deep drawing were carried out. FEM-simulation of the experimentally observed material mechanical behaviour was performed. The variation of the parameters of the stress-strain state in selected areas of the blank volume is shown accounting for the advance of the blank shape transformation.

The reported results could be used to assess of the residual plastic resource of quality steel products, and to investigate and predict the deformation process development in such material. Thus, stability loss during blank form-change or plastic strain localization could be prevented.

Keywords: DEEP DRAWING EXPERIMENTS, FE-MODELING, PLASTIC DEFORMATIONS

1. Introduction

During changing the form of a solid body (metal blank) under the action of the external load together with the evolution of the existing structural defects new ones are initiated, developed and erased [1]. This yields defect transition covering different levels of initiation, accumulation, interaction, combination and coupling, depending on the plastic strain development. As a result, undesired phenomena such as loss of forming stability, plastic strain localization, fracture may occur. They depend on material structure and deformation regimes, i.e. on material plastic resource. Knowing it is of special importance in the design of any deep drawing technology. Pursuing maximal energy and equipment exploitation, a profitable technology is that allowing the fabrication of a piece only by one work travel of the forming tool. Different experimental methods are used to solve that problem, identifying material plastic resource and studying factors that affect blank stability loss and fracture during deep drawing [2].

Due to the complexity of deep drawing factors, it is a rule that the information gained via the best planned and performed experiment is insufficient to describe in detail the drawing process. Hence, numerical simulation is more and more engaged in the field during the last decade, involving material structural characteristics and forming physical and geometrical parameters.

The aim of the present study is to develop a method comprising a physical experiment and numerical modelling, so that material plastic resource could be maximally made use of. To do this, first uniaxial tension test on low-carbon steel bands is carried out to establish precise values of mechanical characteristics. Afterwards with these values, the deep drawing process is numerically modeled under theoretical limiting forming regimes for low-carbon steels in order to find values of limiting parameters of stress strain state at given geometrical sizes of blank and forming stamp. The real physical experiment of deep drawing is performed parallel to numerical simulation.

2. Experimental basis

The good knowledge of the mechanical characteristics of the material is essentially important in design of pieces obtainable by plastic deformation as well as in design of forming tools. For this reason initially uniaxial tension test experiments are carried out. Specimens are strips of low-carbon steel. The dimensions of the specimens are: a length of 150 mm, width 5 mm and thickness 1.5 mm [3]. The “Stress - Strain” diagrams are presented in Fig. 1. Its yield stress is $\sigma_y = 210$ MPa and ultimate strength is $\sigma_u = 440$ MPa. Young’s modulus is $E = 210$ GPa and Poisson’s ratio is $\nu = 0.32$. The mechanical characteristics found are used to design adequate material models and numerically simulate the forming process via the Finite Element Method (FEM).

A series of real physical experiments of deep drawing of low carbon steel were performed in the laboratory. A specially designed deep drawing stamp [4] is fixed to the movable part of a universal testing machine type ZD 10/90 operating in compression. Upon the start of blank deformation an automatic record of the curve “force-travel” also starts in real time, being digitally registered in the computer memory. The stamp parameters are chosen so that to minimize the influence of its design on the material capability to maximal forming. In the specialized handbooks, the maximal ratio of the form-change during deep drawing without blank compromising is varied in the limits $K = D_Z / d = 1.8 \div 2$, where D_Z and d are diameters of blank and piece [1]. The limit blank diameter is calculated as $D_Z = 95.4 - 106$ mm for punch diameter 50 mm and blank thickness 1.5 mm. Theoretically, K is calculated as 2.7 with precondition about proportion of the maximal tensile stresses in the blank material to its ultimate tensile strength higher than 1.1 [5]. That leads to a limit blank diameter of the order of 143.1 mm. The differences, in the range of 10% in the first case and of 25-30% in the second case, give a ground of one more profoundly numerical investigation on the conditions under which the blank material is breaking.

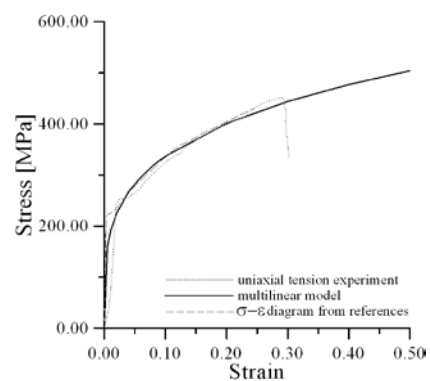


Fig. 1. The true “Stress - Strain” diagram of the investigated low-carbon steel and the corresponding multilinear model.

In this study, an experimental and numerical investigation on the deformation behaviour of blanks possessing diameters 105 mm and 116 mm is presented. The blank diameter $D_Z = 105$ mm is chosen close to the values of the higher admissible limit established and recommended in the practice of sheet metal forming through deep drawing. The blank diameter $D_Z = 116$ mm represents a 10% theoretical increase in the admissible limiting one according to the above precondition concerning the exceeding of material’s tensile strength by the radial tension stresses. Blank thickness is $h_0 = 1.5$ mm, punch diameter is 50 mm, and die diameter is 54 mm at one-side gap of 2 mm. Radii of rounding-off of die and punch are 10 mm and 12 mm respectively.

Fig. 2 shows diagrams “Drawing Force - Work Punch Travel” found experimentally and via numerical simulation. The experimentally found breaking force for blank diameter 116 mm and punch travel 21.4 mm is 9250 N. The drawing force is 7000 N for blank diameter 105 mm and punch travel 20.3 mm. This travel is near to the breaking for the larger blank, but the difference in the force is about 25%. The maximal drawing force is 8600 N for blank diameter 105 mm and punch travel 30 mm. The numerical simulations produced force values of 8400 N, 7218 N and 8283 N, respectively and the differences are 7.02%, 3.02% and 1.37%. The experimentally found current radius of the broken blank is 54.75 mm, while that found via numerical simulation is 54.226 mm. That indicates a presence of developed plastic flow in the blank flange.

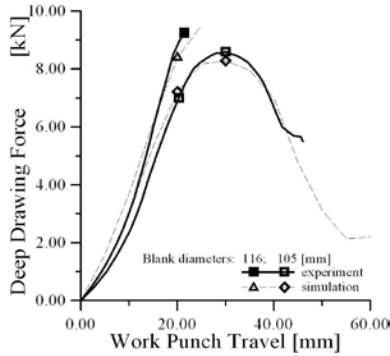


Fig. 2 Experimental and numerical diagrams “Drawing Force - Work Punch Travel”.

Fig. 3a shows the numerically obtained changes of the blank thickness (up) and blank form (down) under punch travel of 20 - 25 mm. Blank thinning in the vicinity of the punch rounding-off is also seen. The blank breaks under punch travel of 21 mm - Fig. 3b.

Based on these comments, a conclusion could be made that the numerical FE model satisfactory describes the forming process and could be used during analyzing the stress strain state of the blanks in the next paragraph.

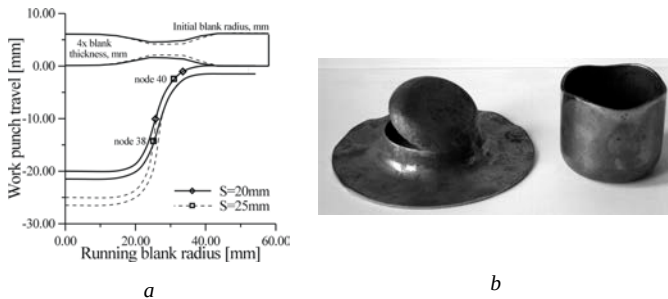


Fig. 3 Blank shapes: numerically (a) and experimentally obtained (b).

3. Finite Element Modeling and Analysis

Deformation and fracture of the steel blank was simulated via FEM using ANSYS software package. Because of symmetry, quarters of the volumes of the two blanks are divided in 651 (Visco107) finite elements with 255 nodes and 777 elements with 300 nodes, respectively for diameters of 105 mm and 116 mm. The process the specific blank holder pressure is 2.47 MPa. The assumed friction coefficients between the blanks and forming tools are 0.16. The forming process is computed in 13 steps for blank diameter 105 mm and punch travel 5 mm per each step. The forming process is computed in 6 steps for blank diameter 116 mm and punch travel 5 mm per each step. With increasing punch travel until 60 mm and until 25 mm, the changes of the two plane blank geometries to cylindrical cup for diameter 105 mm and to fracture for diameter 116 mm are described depending on the distribution of the parameters of the corresponding stress and strain states.

The results are shown in Fig. 4 - Fig. 6. With increasing punch travel forming of cylindrical cup begins under operating of complex stress and strain states. At the beginning of work punch travel the

plastic strains are concentrated in the free of contact area between both radii of rounding-off of die and punch. The blank flange is not in plastic state while the free area begins its transformation in cone enveloping the two radii of rounding-off. Along its contour, the flange is loaded by maximal circumferential pressure stresses and zero radial tension stresses. Following the blank radii from the contour to the centre the radial tension stresses increase and the circumferential compression stresses decrease and become tensional. With increasing travel the flange passes in plastic state, its external diameter (the blank contour) begins to decrease. After the beginning of wall forming, the stresses in the material enveloping the punch radius of rounding-off begin to decrease. The maximal stresses and strains are concentrated in the blank material which envelops the die radius of rounding-off. With the next increase of the punch travel, the transformation of the flange in a wall begins. During this forming the blank wall is loaded at uniaxial tension transmitting the drawing force to the die radius of rounding-off, and blank bottom is loaded under minimal biaxial tension.

Fig. 4 shows the distributions of the stress and strain intensities along the blank radius with diameter 116 mm under punch travel 20 mm. This is the moment immediately before the breaking of the blank. In the area appearing under punch before the rounding-off, the strains are minimal of the order of 0 - 0.043 - 0.086 (Fig. 4a). In the flange they are 0.086 - 0.129. The corresponded stresses are 104 - 156 - 260 MPa and 260 - 364 MPa (Fig. 4b). In the material enveloping the die radius of rounding-off, strain concentrations are read with maximal intensity 0.34 - 0.38 under stress intensity 416 - 460 MPa. Concentrated strain increase of the order of 0.25 - 0.30 - 0.38 is observed in the blank area appearing on the punch radius of rounding-off under stress intensities 380 - 424 - 468 MPa (Fig. 4b). In Fig. 4 and Fig. 6a,b (with red colour), it is seen that in this blank area, a process of plastic strain localization is initiated, because of the suppressed plastic deformation in the flange which is caused by its larger diameter. These localizations (Fig. 3a) with increasing work travel above 20 mm could lead to fracture, as it is happen in Fig. 2 and Fig. 3. The numerical simulation produced a fracture force amounting to 84 kN under punch travel 20 mm. The experiments performed in the laboratory confirmed the observed fracture effects.

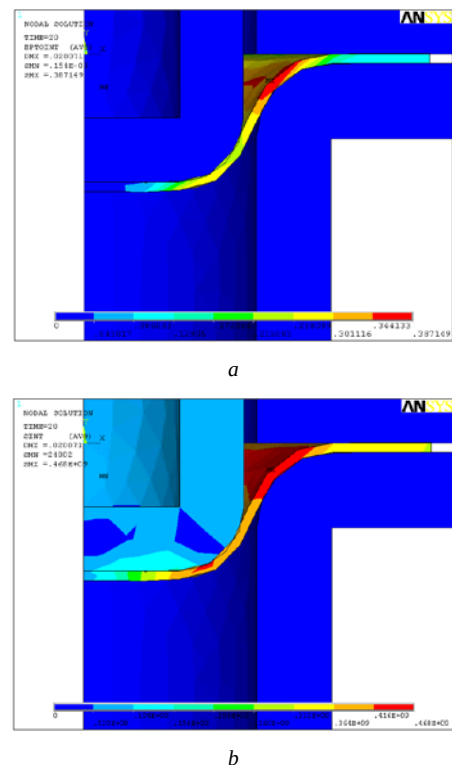


Fig. 4 Strain intensity (a) and stress intensity (b) for deep drawing of a low-carbon steel blank with diameter 116 mm under work punch travel 20 mm.

It is seen that a qualitative piece with diameter 116 mm can not be manufactured. Yet, the results are different when the blank diameter is reduced under the critical value of 105 mm. Under the same work punch travel of 20 mm, stresses amounting to 220 - 275 - 330 MPa occur and deformation with intensity 0.101 - 0.152 - 0.203 is attained (Fig. 5).

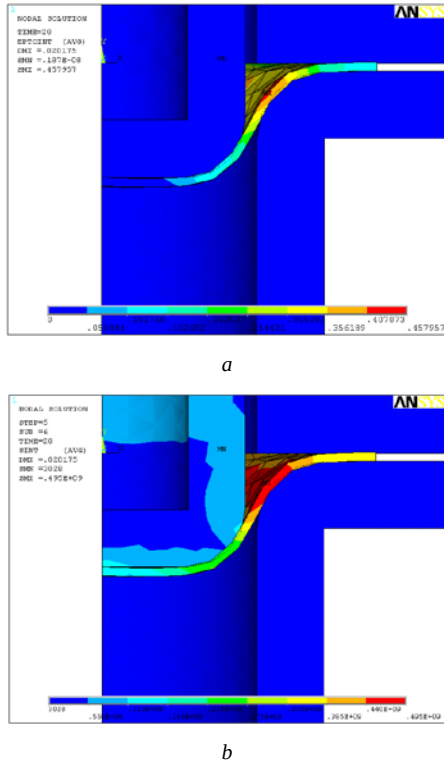


Fig. 5 Strain intensity (a) and stress intensity (b) for deep drawing of a low-carbon steel blank with diameter 105 mm under work punch travel 20 mm.

The piece height (Fig. 6c,d) obtained by the simulation is 44.48 mm, and the experimentally measured is variable 43 - 46 mm due to the anisotropy (Fig 3b).

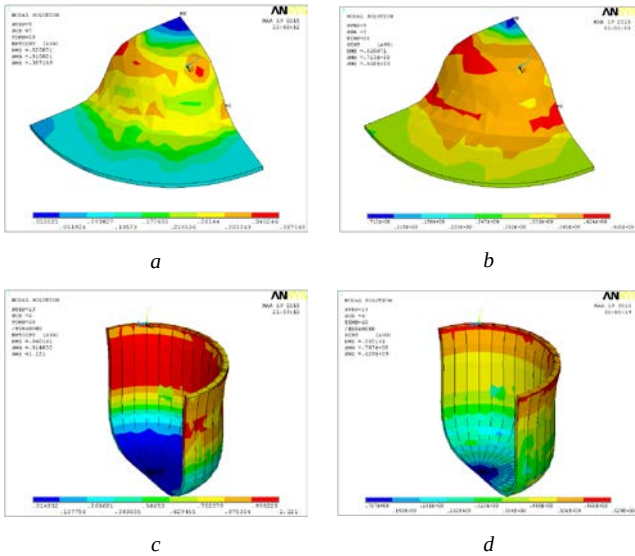


Fig. 6 Strain and stress distributions of the of a blank with diameter 116 mm before fracture at punch travel 20 mm (a, b) and of a blank with diameter 105 mm at punch travel 60 mm (c, d) at the end of the forming process.

In difference from the larger diameter, here in the central blank area which is below the punch, the strains are minimal, little bit over the theoretical plastic strain limit of 0.02, in the range of 0 - 0.05 (Fig. 5a). In the blank flange the strains are in the range of 0.152 - 0.2 - 0.254, almost two times more intensive than the observed in the previous case, i.e. a developed plastic flow appears

in the flange. The corresponded stresses in the bottom and the flange are 110 - 165 MPa, far below the yield stresses and significantly over them in the range of 330 - 385 MPa (Fig. 5b). The concentrated strains in the blank material which appears on the die rounding-off are also more intensive in the ranges of 0.356 - 0.4 - 0.457 under stresses of 385 - 440 - 495 MPa. Strain intensity in the blank material covering the punch rounding-off is almost two times lower 0.1 - 0.15 - 0.2, and the stresses are also lower 220 - 275 MPa. Based on these numerical data, the conclusion is imposed that the blank with diameter 105 mm is more favourably loaded. The material continuity is saved under stability of the changes in the blank form according to this assigned by the forming tool.

Under maximal drawing force of 83 kN punch travel of 30 mm, the stress intensity at the punch rounding-off is 257 - 322 MPa, while strain intensity is 0.095 - 0.190 - 0.285. The blank does not break, while the final product is shown in the right of Fig. 3b. The increasing strains from minimal elastic in the bottom to maximal plastic along the height of the wall are seen. The formed cup is produced by the transformation of the flange of blank with diameter 105 mm into the cup wall under stresses in the ranges of 445 - 506 - 568 MPa. That is caused by the punch work travel larger than 25 mm when both the radii of rounding-off of die and punch are enveloped by the blank material.

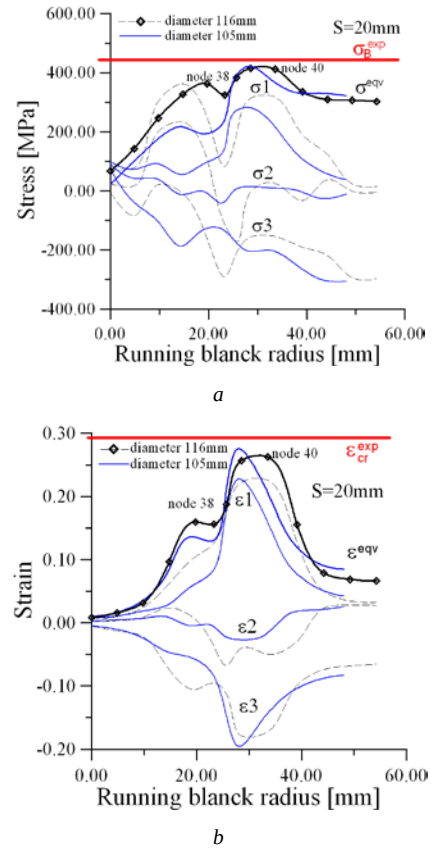


Fig. 7 Principal stress and strain distribution along the blank current radius.

The distributions of the principal stresses and strains along the blank radius are shown in Fig. 7. The effect of the strain concentration in the free of contact area is clearly seen. With diameter 116 mm for current blank radius between 10 and 20 mm, the maximal principal radial stresses σ_1 approach the uniaxial tensile strength σ_B of the blank material (Fig. 1). After this area they decrease and break the material (Fig. 2 and Fig. 3), with sharp increase of the stains in elements 38 and 40 (Fig. 7b), and increasing punch travel from 20 mm to 25 mm (Fig. 8). With blank diameter 105 mm the stresses operating in the same area have lower values, fracture is not obtained. Here, the principal negative circumferential compression stresses σ_3 have absolutely maximal values, while with the larger diameter 116 mm, here, the compression circumferential stresses increase sharply from 0 to

absolute (compression) maximum. At the expense of that, the tension along the thickness increases with increasing radial tension which leads to thinning and next breaking (Fig. 9). With diameter 105 mm the stresses along the thickness are close to zero. The conclusion follows that increase of the blank diameter leads to suppression of the plastic flow development in the flange which causes an exchange in the roles of the thickness stresses and circumferential stresses. This phenomenon produce thinning and breaking with the larger diameter, and with the smaller diameter envelopment of the punch roundness radius by the blank material subjected to circumferential compression stresses, keeping the thickness and establishment of favourable conditions for transmitting the drawing force by the wall to the flange. In our opinion, the differences between the uniaxial tensile strength σ_B^{exp} and fracture strain $\varepsilon_{\text{cr}}^{\text{exp}}$ and the corresponding equivalent stresses σ^{eqv} and strains ε^{eqv} numerically identified on the experimental basis represent remained plastic resource which is consumed with increasing punch travel to 25 mm.

Fig. 8 shows the distribution of the principal stress and strain obtained for the larger blank in nodes 40 and 38 belonging to the upper blank surface and possessing initial radii 38.66 mm and 29.0 mm and current radii 30.95 mm and 25.68 mm. These are the stress and strain history in the broken blank area.

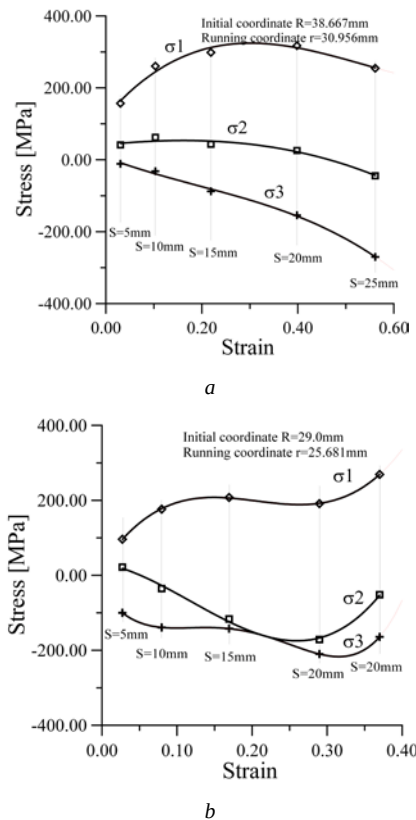


Fig. 8 Development of the principal stresses in the fracture area.

The first node is chosen in the middle of the flange and the second is chosen in the middle of the area initially appearing over the die rounding-off. It is seen that in the two nodes (as well as, in the area between them, and also, in a ring blank area possessing initial radii around and over them) with increasing punch travel from 0 to 5 mm there are no developed plastic strains. That also shows concentrations of the strains in the areas with smaller initial radii between both radii of rounding-off. The plastic flow in the ring defined by the two radii is initiated after punch travel 10 mm. At the first node with the increasing travel from 15 to 20 mm the principal strains are increased from 0.2 to 0.4, and at the second node they are smaller from 0.17 to 0.30, but there the increase is almost in two times. At the first node, the stress state is constant tension/increasing circumferential compression/minimal thickness tension. At the second node, similar stress state in radial and circumferential directions is seen, but under lower tension values close to these of

uniaxial yield stresses. Here, the difference is that the compression load along the thickness is almost commensurable to this in the circumferential direction. This is the area with initial radius 29 mm, in which with increasing punch travel to 25 mm follows a sharp increase of the maximal principal tension radial stress (Fig. 8b) sharp increase of strain intensity (Fig. 7b) and strain localization and breaking is obtained finally (Fig. 3b, Fig. 6a,b).

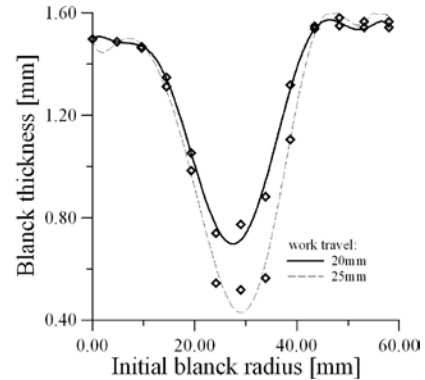


Fig. 9 Blank thickness before and during breaking with travel 20 - 25 mm.

4. Conclusion

Considering deep drawing, the stressed state varies in different blank areas (Fig. 4 - Fig. 6). This yields different degree of material strain-hardening and as a result-different carrying capacity (Fig. 7). Here, the initial blank diameter has an essentially important significance, because its size combined with its mechanical material's characteristics (Fig. 1) determines the flange resistance against the change of its form into a piece wall trough plastic deformation. Hence, good knowledge on the material characteristics and the variation of the stressed and strained states is needed to predict material mechanical behaviour and make maximal use of its plastic resource. From point of view fracture mechanics, the processes developed in fractured blank area (Fig. 8 and Fig. 9) could be investigated more particularly by the concentration of both the methods experimental observation and numerical modeling in such an area as the identified here, its stress strain state, possible structural changes and prevailing mechanisms of plastic deformation.

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SPECKLE PATTERN INTERFEROMETRY FOR MEASUREMENT OF RESIDUAL STRESS: BASIC APPROACH, MATHEMATICAL SUPPORT, SPECIAL ARRANGEMENT, PRACTICAL APPLICATION

СПЕКЛ-ИНТЕРФЕРОМЕТРИЯ ДЛЯ ОПРЕДЕЛЕНИЯ ОСТАТОЧНЫХ НАПРЯЖЕНИЙ: ОБЩИЙ ПОДХОД, МАТЕМАТИЧЕСКОЕ ОБЕСПЕЧЕНИЕ, СПЕЦИАЛЬНОЕ ОБОРУДОВАНИЕ, ПРАКТИЧЕСКОЕ ПРИМЕНЕНИЕ

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Abstract. The paper provides a comprehensive description of theoretical and practical aspects of electronic speckle pattern interferometry for technological residual stress measurement in various machine elements. Any results obtained by investigation of residual stress in a welded joint are presented.

KEYWORDS: SPECKLE, INTERFEROMETRY, DISPLACEMENTS FIELD, RESIDUAL STRESS, HOLE DRILLING, DEFORMATION RESPONSE, MATHEMATICAL INTERPRETATION, WELDED JOINT

1. Introduction

Information about levels and distribution of technological residual stress in materials is an important condition to guarantee strength and resource of machine structure [1, 2]. This is of utmost importance for structural elements with welded joints. In the vast majority of cases this information is received experimentally using destroying or partially destroying procedures. The current engineering practice mainly uses small hole drilling as stress indicators. The procedure for wide processing of source experimental data in terms of stresses is in fact an inverse problem of mechanics of deformable solids. Components of residual stress tensor are calculated basing on records of material local strain response in the drilling area using an adequate mathematical model. Various experimental mechanical equipment is used to measure strain response, including tensor resistant transformer sockets. However in this case the investigator receives but minimal information for analysis. Recent advanced trend is based on use of contactless coherent optical methods to perform high accuracy measurements of full displacement fields in the entire surface area of the deformable body [3, 4].

2. Preconditions and means for resolving the problem

Electronic speckle-pattern interferometry is the most effective optical method in analysis of residual stress [5 - 8]. Recording and further use of strain response in the form of fields of two mutually orthogonal tangential components of displacements u and v is a preferred option from the standpoint of reliability of stress component measurement. To measure each of the component the object is illuminated simultaneously with two wide laser beams that are symmetrical with respect to normal OZ to its surface and lying in the same surface with the axis of displacements under measurement (direction of sensitivity of individual interferometers), i.e. OX or OY respectively. Figure 1 demonstrates an optical configuration for the measurement of displacement component u .

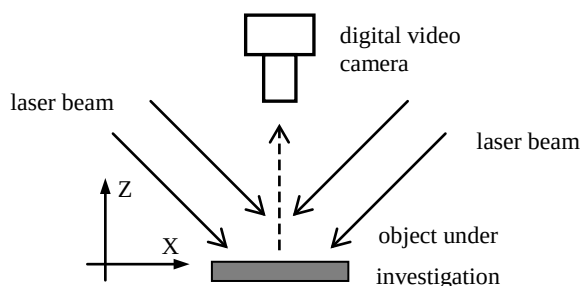


Figure 1. Optical scheme of a speckle-pattern interferometer to measure displacement vector tangential component.

Images of the object before and after hole drilling are recorded using a digital video camera, transferred to the computer and stored as digital files. Primary information processing involves pairwise subtraction of digitized shots as recorded in each of the configurations and reflecting two different states of the object. As a result the difference images are covered by systems of bands which are lines of equal displacements u or v respectively. Pointwise decoding of the band pictures is made using the following relationships:

$$u = N_1 \frac{\lambda}{2 \sin \alpha}; \quad v = N_2 \frac{\lambda}{2 \sin \alpha} \quad (1)$$

where N_i is the fringe order in different points in respective interferograms (fringe patterns), λ is laser wave length (λ is about $0.5 \mu\text{m}$), α is the illuminating beam direction angle.

Importantly, the recorded pictures themselves do not carry information about displacement signs which is characteristic of all optical interference methods. Identification of u and v signs involves inclusion by optical means of an additional known phase displacement of the illuminating light waves and analysis of the resulting changes in fringe pattern. In particular, additional linear phase displacement may be achieved by a slight inclination of the illumination beams towards the normal OZ . In the absence of displacements on the body surface this inclination induces interferograms as parallel equidistant bands oriented along the OY axis in case of the u measurement configuration, or the OX axis in case of the v measurement configuration. The picture in the indicator hole drilling area undergoes transformation and acquires a characteristic pattern depending on displacement signs. Below are shown typical interferograms as observed in study of values and signs of residual stresses using the hole drilling technique. Band pictures in Figures 2a and 2b characterize fields of displacement component u (horizontal for this picture orientation) as observed with different ratios of main residual stresses, corresponding with laboratory axes OX and OY in this case. Interferograms observed after inclusion of an additional linear phase displacement into illumination beams are used to identify signs of displacement (Figures 2c and 2d respectively). If sign of this displacement is known, it is easy to determine sign of the measured displacements by simple analysis of these fringe patterns. The main point here is to find out whether one should add or subtract phase displacements that are caused artificially by moving the body surface. This determines the side of inclination of the equidistant band raster that characterizes the additional phase displacement only. Analysis of interferograms in the cases considered helps to determine directions of displacements that are marked with arrows in the figures.

Figure 3 is an example of measurement of displacement component v , when the unknown main axes of stress state and the laboratory axes do not coincide. In such cases the observed fringe patterns are

not as a rule symmetrical, however their decoding procedure and the rule for identification of displacement signs remain the same.

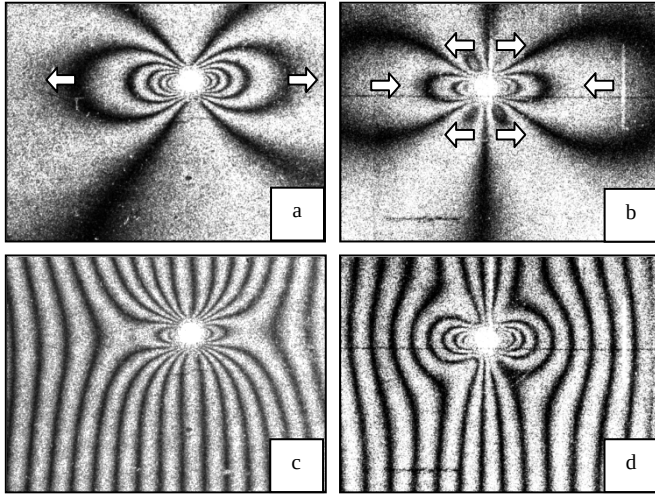


Figure 2. Typical interferograms of displacement fields in the vicinity of holes drilled in a body with residual stresses: a, b — initial interferograms; c, d — interferograms after inclusion of an additional linear phase displacement into illuminating beams.

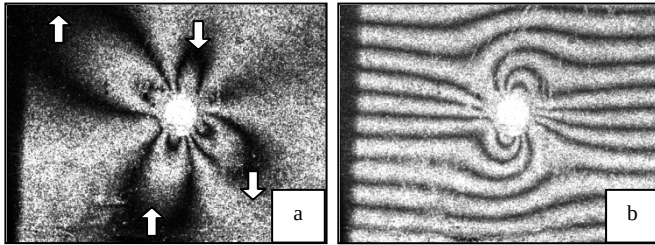


Figure 3. Typical interferograms in case of misalignment of the interferometer sensitivity axis and the main axis of residual stresses in the body.

3. Solution of the examined problem

The procedure for wide processing of experimental information in terms of residual stress components consists in minimization of deviations between recorded displacement fields and theoretically expected distributions as calculated basing on a mechanical model with variable stress state parameters. According to the commonest engineering approaches the analysis is made in the approximation of exclusively elastic deformation with stresses within the minor drilling area are assumed homogeneous. In study of thin-wall structural elements and indicator through-hole drilling the model for expected response is based on the well-known analytical solution of the Kirsh problem. In case of massive structures with blind holes drilled to the preset depth on their surfaces nominal response functions in displacements are found by finite element method.

Let the model displacement functions expected after hole drilling in the presence of a single stress $\sigma_x = 1$ ($\sigma_y = 0$) as obtained by some method are $u_1 = f(r, \varphi)$ and $v_1 = g(r, \varphi)$. Here r, φ are polar coordinates of an object point in a system with the beginning in the hole center. Then calculation of stress state parameters ($\sigma_x, \sigma_y, \tau_{xy}$) in the minor drilling area is made by solution of the system of linear equations

$$\sigma_x f(r, \varphi) - \sigma_y g\left(r, \varphi - \frac{\pi}{2}\right) + \tau_{xy} h_1 \frac{\sqrt{2}}{2} + u_0 = u \quad (2a)$$

$$\sigma_x g(r, \varphi) + \sigma_y f\left(r, \varphi - \frac{\pi}{2}\right) + \tau_{xy} h_2 \frac{\sqrt{2}}{2} + v_0 = v \quad (2b)$$

$$h_1 = f(r, \varphi_1) + f(r, \varphi_2) - g(r, \varphi_1) + g(r, \varphi_2)$$

$$h_2 = f(r, \varphi_1) - f(r, \varphi_2) + g(r, \varphi_1) + g(r, \varphi_2)$$

$$\varphi_1 = \varphi - \frac{\pi}{4}; \quad \varphi_2 = \varphi - \frac{3\pi}{4}$$

containing on the right side actual displacement values measured by interferograms of displacement fields u and v respectively in M_1 and

M_2 points situated in dark fringes. Most stable results are achieved with the choice of points at a distance of 2 to 5 radii from the hole center. Additional unknown model parameters u_0 and v_0 are included in equations (2a)-(2b) to allow for a possible unpredictable displacement of the object as a rigid whole with respect to the measuring system. The speckle pattern interferometry technique allows measurement of displacements in a rather large number of points, i.e. $M = M_1 + M_2 > 5$. Therefore the system of equation (2) is considered overdetermined and is solved by the least square method. This approach reduces significantly the effect of experimental errors. Then, if needed, the investigator addresses main stresses σ_1, σ_2 and angle of orientation of main axes basing on values of stress state components in the laboratory coordinate system OXY.

Note that according to formulae (1) speckle-pattern interferometry sensitivity threshold in displacements is several tenths of micrometer. If maximal fringe orders in interferograms after indicator hole drilling do not exceed 1, then calculation of stresses with the approach considered becomes problematic. However this task remains soluble within certain limits if results of interferogram decoding obtained after inclusion of additional linear light beam phase displacement are used as source data. Obviously in this case that model presentations should also contain linear terms such as $A \cdot x = A \cdot r \cdot \cos(\varphi)$ for equations (2a) and $B \cdot y = B \cdot r \cdot \sin(\varphi)$ for equations (2b). Constants A and B are additional parameters of the extended model and are also considered generally unknown. The number of experimental points should be increased accordingly, i.e. $M > 7$. Estimated sensitivity threshold for the method of residual stress measurement in this case is about $(1.5 \div 2) \cdot 10^{-4} E$, where E is Young's modulus.

After calculation of main ($\sigma_x, \sigma_y, \tau_{xy}$) and additional (u_0, v_0, A, B) model parameters it is reasonable to solve the direct problem with imitation of interference fringes. If these patterns reproduce actual interferograms with a high accuracy, one may make judgments about adequacy of the obtained results. Figure 4 is an example of actual interferograms recorded experimentally with model fringes as thin white lines superimposed. As seen, high quantitative and qualitative coincidence of the bands is observed in this case.

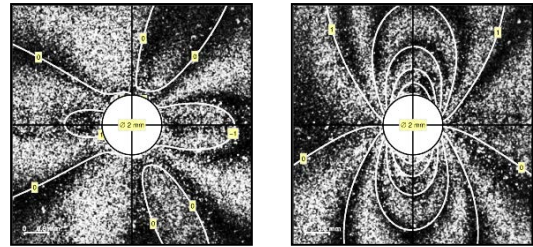


Figure 4. Comparison of actual interferograms with model displacement field isolines.

Experimental study of residual stresses in samples at this stage of testing of technological production modes of structural elements is made under laboratory conditions using special optical arrangement (Figure 5a). A series of measuring instruments is developed for full-scale testing of objects at various stages of their manufacture [9, 10] (Figure 5b). High structural rigidity is the main requirement for such equipment. Compactness of portable interferometers is ensured by small-size components, i.e. the laser and the video camera, as well as by a simple optical configuration as shown in Figure 6.

4. Results and discussion

Detection of residual stress in weld-fabricated structures is an important problem to be solved using the approaches and equipment developed. In particular, of much importance is information about the presence and levels of residual stresses in welded pipe-lines [11, 12]. Figure 7 shows results of study of a pipe-line element with a ring welded joint as an example. x-coordinates in the diagrams correspond with axis coordinates of hole drilling points as counted from the joint center. As seen, stresses in the thermal effect area may reach rather high values which produces a negative impact on general strength characteristics of the structure and should be taken into account in assessment of its exploitation durability.

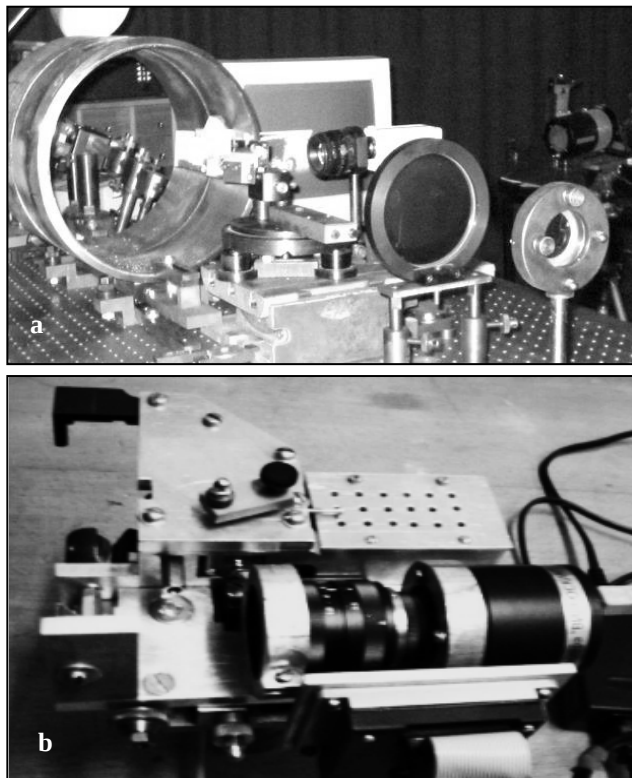


Figure 5. Experimental equipment for laboratory (a) and nonlaboratory (b) studies.

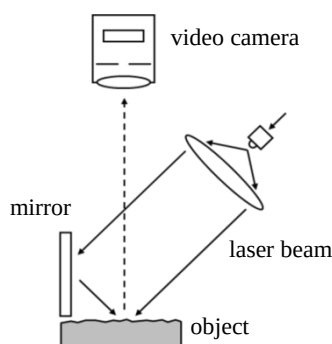


Figure 6. Simplified optical interferometer scheme for tangential displacement measurement.

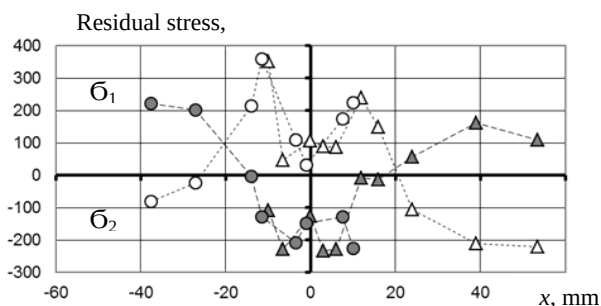


Figure 7. Distribution of components of residual stress tensor.

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5. Conclusion

Electronic speckle-pattern interferometry is an effective tool to study residual stresses in samples and actual structural elements of industrial objects. Of the most practical utility is its combination with drilling of small-size holes as indicators of type and level of the body stress state. Development of special autonomous measuring equipment allows the whole complex study to be conducted under ex-laboratory conditions.

MEASURING CONTACT PRESSURES BY METHOD CORRELATION SPECKLE PHOTOGRAPHY

ИЗМЕРЕНИЕ КОНТАКТНЫХ ДАВЛЕНИЙ МЕТОДОМ КОРРЕЛЯЦИОННОЙ СПЕКЛ ФОТОГРАФИИ

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Abstract: A method for measuring contact pressures based on the measurement of irreversible changes in a surface microrelief by the speckle photography technique is presented. The analytic dependence between the change in the contrast of the carrying Young's fringes and the relative area of change in the microrelief is considered. An example of a contact interaction between a cylinder end and a flat slab, the latter with a specially produced regular roughness on its contact surface, is used to experimentally verify the relation between the irreversible change in the roughness, the change in the contrast of the holographic interference fringes, and the change in the contrast of the carrying Young's fringes. It is shown that the sensitivity of correlation speckle photography is higher than the sensitivity of the correlation holographic interferometry technique.

KEYWORDS: CONTACT PRESSURES, METHOD CORRELATION SPECKLE PHOTOGRAPHY, FRINGE CONTRAST.

1. Introduction

The decrease in the fringe contrast in the speckle photography method that is caused by an irreversible change in the surface microrelief of an object can be used to solve various problems of contact-interaction mechanics [1-3], among which the possibility of contact-pressure measurements should be distinguished. To solve this problem, as a rule, intermediate bodies that are introduced directly into the contact zone of two bodies are currently used. The values of the contact pressures are estimated by measuring the hardness in the contact zone of the plastically strained spacer [4]. A film of a liquid-crystal substance is sometimes used as the spacer, and the contact pressures are evaluated by changes in the colors of the spacer's regions [5, 6]. However, the presence of bodies in the contact zone leads to modification of the conditions of the contact interaction and, as a result, to an increased error in contact-pressure measurements. Below, we consider a method of contact-pressure measurements based on the recording of irreversible changes in the surface microrelief of a body using the speckle photography technique. A theoretical dependence between the change in the contrast of the carrying Young's fringes and the relative area of change in the microrelief is established. This relation is experimentally verified using the example of the contact between an end of a hard cylinder and a flat slab.

2. Principle of the method

Let a speckle structure of an image of a studied flat surface of a body illuminated by coherent light be recorded on a photographic plate during the first exposure. Subsequently, contact interaction of the bodies under investigation is effected. The photographic plate is then displaced in its plane by a value equal to a few average cross-sectional dimensions of a speckle. Then, another speckle structure of the body's surface image is recorded (the second exposure). When the resulting twice-exposed speckle photograph is illuminated with a nonexpanded laser beam, parallel fringes are observed in the frequency plane. The period and orientation of these fringes are determined by the vector of displacement of the photographic plate between the exposures. However, for those regions of the speckle photographs that correspond to the body's surface areas, where, as a consequence of the contact interaction, irreversible changes in the microrelief have occurred, the contrast of fringes decreases. Thus, plastic strain of elements of the microrelief of the body's surface leads to a decorrelation of the speckle structures of the body's surface images and, consequently, to a reduced contrast of the interference fringes. An example of a contact interaction between a cylinder end and a flat slab, the latter with a specially produced regular roughness on its contact surface,

is used to experimentally verify the relation between the irreversible change in the roughness, the change in the contrast of the holographic interference fringes, and the change in the contrast of the carrying Young's fringes. It is shown that the sensitivity of correlation speckle photography is higher than the sensitivity of the correlation holographic interferometry technique [5].

Let $E(\omega)$ be the light intensity in the frequency plane and

$$E(\omega) = \left\langle |F(\omega)|^2 \right\rangle, \quad (1)$$

where ω is the radius vector in the frequency plane, $F(\omega)$ is the complex amplitude of the field in the frequency plane, and $\langle \dots \rangle$ is the averaging operation. Assuming the photorecording process to be linear up to a constant, we can write that

$$F(\omega) = \int I(\mathbf{r}) \exp[i(\omega \mathbf{r})] d\mathbf{r}, \quad (2)$$

where $\mathbf{r}$ is the radius vector in the plane of the speckle photography, $I(\mathbf{r}) = I_1(\mathbf{r}) + I_2(\mathbf{r})$, and $I_1(\mathbf{r})$ and $I_2(\mathbf{r})$ are the light intensities in the plane of the photographic plate during the first and second exposures, respectively. The integration in (2) is performed over the area of the photographic plate illuminated by the laser beam. Substituting expression (2) into (1), we obtain

$$E(\omega) = \left\langle I(\mathbf{r}_1) I(\mathbf{r}_2) \right\rangle \exp[i\omega(\mathbf{r}_1 - \mathbf{r}_2)] d\mathbf{r}_1 d\mathbf{r}_2. \quad (3)$$

The correlation of the intensities in (3) can be written as

$$\begin{aligned} \left\langle I(\mathbf{r}_1) I(\mathbf{r}_2) \right\rangle &= \left\langle I_1(\mathbf{r}_1) I_1(\mathbf{r}_2) \right\rangle + \left\langle I_1(\mathbf{r}_1) I_2(\mathbf{r}_2) \right\rangle + \\ &+ \left\langle I_2(\mathbf{r}_1) I_1(\mathbf{r}_2) \right\rangle + \left\langle I_2(\mathbf{r}_1) I_2(\mathbf{r}_2) \right\rangle, \end{aligned} \quad (4)$$

where $I_j(\mathbf{r}) = |V_j(\mathbf{r})|^2$ ($j=1,2$) and $V_j(\mathbf{r})$ are the complex field amplitudes in the plane of the speckle photograph during the first and second exposures.

Now, let $U_j(\xi)$ be the complex field amplitudes in the plane of the object under study; then,

$$V_j(\mathbf{r}) = \int_{S_0} U_j(\xi) h(\xi - \mathbf{r}) d\xi \quad (5)$$

where $h(\xi - \mathbf{r})$ is the pulse response of the image-forming lens,

S_o is the area of the resolved element, and ξ is the vector in the plane of the surface under study. The fourth-order correlation moments of the complex amplitude in formula (4) for a random Gaussian process are expressed through second-order moments. For example, for the first term of the right-hand side of (4), we have

$$\begin{aligned} \langle I_1(\mathbf{r}_1) I_1(\mathbf{r}_2) \rangle &= \langle I_1(\mathbf{r}_1) \rangle \langle I_1(\mathbf{r}_2) \rangle + \\ &+ \left| \langle V_1(\mathbf{r}_1) V_1^*(\mathbf{r}_2) \rangle \right|^2. \end{aligned} \quad (6)$$

The average intensities are $\langle I_i(\mathbf{r}_j) \rangle$, ($j=1,2$):

$$\langle I_i(\mathbf{r}_j) \rangle = \int \langle U_j(\xi_1) U_j^*(\xi_2) \rangle h(\xi_1 - \mathbf{r}) h(\xi_2 - \mathbf{r}) d\xi_1 d\xi_2.$$

The δ -correlated amplitude is

$$\langle U_j(\xi_1) U_j^*(\xi_2) \rangle \sim \delta(\xi_1 - \xi_2), \quad (j=1,2).$$

With allowance for the last term on the right-hand side of Eq. (6),

$$\begin{aligned} \langle I_j(\mathbf{r}) \rangle &= \int_{S_o} |h(\xi - \mathbf{r})|^2 d\xi \sim S_o, \quad (j=1,2), \\ \langle V_1(\mathbf{r}_1) V_1^*(\mathbf{r}_2) \rangle &\sim \int_{S_o} h(\xi - \mathbf{r}_1) h^*(\xi - \mathbf{r}_2) d\xi \sim S_o h(\mathbf{r}_1 - \mathbf{r}_2) \end{aligned}$$

The latter expression is derived taking into account the fact that the pulse response is proportional to the Fourier transform of the aperture of the objective. The final expression for (6) takes the form

$$\langle I_1(\mathbf{r}_1) I_1(\mathbf{r}_2) \rangle \sim S_o^2 \left(1 + |h(\mathbf{r}_1 - \mathbf{r}_2)|^2 \right). \quad (7)$$

It is easy to show that the latter term in (4) has an identical expression, i.e.,

$$\langle I_2(\mathbf{r}_1) I_2(\mathbf{r}_2) \rangle = \langle I_1(\mathbf{r}_1) I_1(\mathbf{r}_2) \rangle. \quad (8)$$

The second term on the right-hand side of (4) is written in the form

$$\begin{aligned} \langle I_1(\mathbf{r}_1) I_2(\mathbf{r}_2) \rangle &= \langle I_1(\mathbf{r}_1) \rangle \langle I_2(\mathbf{r}_2) \rangle + \\ &+ \left| \langle V_1(\mathbf{r}_1) V_2^*(\mathbf{r}_2) \rangle \right|^2. \end{aligned} \quad (9)$$

The complex amplitudes in (9) are represented as a sum

$$\begin{aligned} V_1(\mathbf{r}_1) &= \int_S U_1(\xi) h(\xi - \mathbf{r}) d\xi + \int_F U_1(\xi) h(\xi - \mathbf{r}) d\xi = \\ &= V_{1S}(\mathbf{r}_1) + V_{1F}(\mathbf{r}_1), \end{aligned} \quad (10)$$

where S is the area of the surface with an unaltered microrelief and F is the surface area with the microrelief randomly altered as a result of the contact interaction. It is obvious that $S + F = S_o$. The

complex amplitude $V_2^*(\mathbf{r}_2)$ can be represented in a similar form:

$$V_2^*(\mathbf{r}_2) = V_{2S}^*(\mathbf{r}_2) + V_{2F}^*(\mathbf{r}_2). \quad (11)$$

Substituting (10) and (11) into (9) and taking into account that

$$\langle V_{1S}(\mathbf{r}_1) V_{2F}^*(\mathbf{r}_2) \rangle = \langle V_{1F}(\mathbf{r}_1) V_{2S}^*(\mathbf{r}_2) \rangle = 0,$$

we obtain

$$\begin{aligned} \langle V_1(\mathbf{r}_1) V_2^*(\mathbf{r}_2) \rangle &= \langle V_{1S}(\mathbf{r}_1) V_{2S}^*(\mathbf{r}_2) \rangle = \\ &= \int \langle U_1(\xi_1) U_1^*(\xi_2) \rangle h(\mathbf{r}_1 - \xi_1) h^*(\mathbf{r}_2 - \xi_2 - \mathbf{d}) d\xi_1 d\xi_2, \end{aligned} \quad (12)$$

where $\mathbf{d}$ is the vector of displacement of the photographic plate between the exposures. Formula (12) was derived using the expression

$$V_{2S}^*(\mathbf{r}_2) = V_{1S}^*(\mathbf{r}_2 + \mathbf{d}).$$

By analogy with the derivation of relation (7), it can be deduced that

$$\langle I_1(\mathbf{r}_1) I_2(\mathbf{r}_2) \rangle \sim S_o^2 + S^2 |h(\mathbf{r}_1 - \mathbf{r}_2 - \mathbf{d})|^2. \quad (13)$$

For the third term on the right-hand side of (4), we have

$$\langle I_2(\mathbf{r}_1) I_1(\mathbf{r}_2) \rangle \sim S_o^2 + S^2 |h(\mathbf{r}_1 - \mathbf{r}_2 + \mathbf{d})|^2. \quad (14)$$

Substituting expressions (7), (8), (13), and (14) into (4), we obtain

$$\begin{aligned} \langle I(\mathbf{r}_1) I(\mathbf{r}_2) \rangle &\sim 4S_o^2 + 2S_o^2 |h(\mathbf{r}_1 - \mathbf{r}_2)|^2 + \\ &+ S^2 |h(\mathbf{r}_1 - \mathbf{r}_2 - \mathbf{d})|^2 + S^2 |h(\mathbf{r}_1 - \mathbf{r}_2 + \mathbf{d})|^2. \end{aligned} \quad (15)$$

Using (15), it is easy to show that the intensity distribution in the frequency plane according to (3) is

$$E(\omega) \sim 4S_o^2 \delta(\omega) + 2\Phi(\omega) [S_o^2 + S^2 \cos(\omega \mathbf{d})], \quad (16)$$

where $\delta(\omega)$ is the delta function describing a bright point in the

frequency plane and $\Phi(\omega) = \int |h(\mathbf{R})|^2 \exp(i\omega \mathbf{R}) d\mathbf{R}$ is the autocorrelation function of the frequency spectrum of the lens forming the image of the surface investigated. For a lens with a circular aperture, $\Phi(\omega)$ is the autocorrelation function of a circle. Excluding the bright point in the frequency plane by using spatial filtering (see (16)), we finally obtain

$$E(\omega) \sim \Phi(\omega) \left[1 + \frac{S^2}{S_o^2} \cos(\omega \mathbf{d}) \right]. \quad (17)$$

It follows from (17) that the contrast of the fringes that modulate the autocorrelation function $\Phi(\omega)$ is

$$\gamma_S = \frac{S^2}{S_o^2} = \left(1 - \frac{F}{S_o} \right)^2. \quad (18)$$

Hence, according to formula (18), a change in the contrast γ_S of fringes in the frequency plane allows one to estimate the fraction of the contact surface on which an irreversible change in the body's surface microrelief took place:

$$\frac{F}{S_o} = 1 - \sqrt{\gamma_S}. \quad (19)$$

Note that formula (19) is valid under the condition that the size of the diffraction halo determined by the function $\Phi(\omega)$, substantially exceeds the period T of the modulation fringes in the frequency plane; i.e.,

$$D \gg T = \frac{\lambda f}{d},$$

where D is the diameter of the lens forming the surface image and f is the distance from the speckle photograph to the frequency plane. It is also assumed that the dimensions of the illuminated area of the twice-exposed speckle photograph are small enough, and it can be considered that the irreversible change in the microrelief on the corresponding area of the contact surface is constant. In the first approximation, the change in the contrast of the holographic carrying fringes γ_H is equal to the ratio of the area F of the plastic component of the contact surface to the area S_o of the contour surface of the contact:

$$\gamma_H = 1 - \frac{F}{S_0} \quad (20)$$

Comparing expressions (18) and (20) results in the following known equation [3]:

$$\gamma_S = \gamma_H^2 \quad (21)$$

In other words, for one and the same irreversible change in the body's surface microrelief, the process of decorrelation of the speckle structure has a higher rate than the decorrelation of the light waves reconstructed using the twice-exposed hologram. Expression (21) is obtained under the condition that the carrying fringes have a contrast equal to unity. In practice, the contrast of these fringes is always less than unity. This should be taken into account in normalizing the change in the contrast of the carrying fringes:

$$\frac{\Delta\gamma}{\gamma_o} = \frac{\gamma_o - \gamma}{\gamma_o} \quad (22)$$

where γ_o is the contrast of the carrying fringes outside the zone and γ is the contrast of the carrying fringes at the measurement point contact. In view of (22), relation (21) takes the form

$$\frac{\Delta\gamma_S}{\gamma_{oS}} = 2 \frac{\Delta\gamma_H}{\gamma_{oH}} - \left(\frac{\Delta\gamma_H}{\gamma_{oH}} \right)^2 \quad (23)$$

3. Experimental results

The theoretical relationships obtained were verified on the example of the contact between an end of a rigid steel cylinder 15 mm in diameter with a roughness $R_a = 0.32 \mu\text{m}$ and a flat slab made of D16T material. A regular microrelief in the form of grooves and ridges with the roughness parameter $R_a = 6.5 \mu\text{m}$ was applied to the slab surface. A typical profilogram of the initial microrelief obtained with a Kalibr-252 profilograph is shown in Fig. 1a, where the horizontal and vertical magnifications are 20 and 1000, respectively. Holograms and speckle photographs of the slab surface under study were recorded simultaneously using the optical system described in [2]. In each experiment, a profilogram of the surface microrelief was recorded along the diameter of the contact zone. For this purpose, the slab was precisely fixed using a special kinematic device both when the photograph was taken and when the surface microrelief was recorded before and after the contact interaction. Thus were profilograms over one and the same cross section of the contact surface recorded. A profilogram of the slab surface microrelief after contact with a cylinder end at a load of 20 kN is shown in Fig. 1b. Comparing the profilograms obtained for one and the same cross section (Fig. 1) makes it possible to clearly visualize the contact boundary and the change in the heights of the surface microrelief. In view of the fact that, in the case considered, we deal with a regular roughness and plastic strain of the roughness develops from its top, the relative change in the contrast of the carrying holographic fringes in (20) and (21) can be considered equal to the irreversible relative change in the roughness height:

$$\frac{\Delta\gamma_H}{\gamma_{oH}} = 1 - \frac{h}{H} = \frac{\Delta h}{H} \quad (24)$$

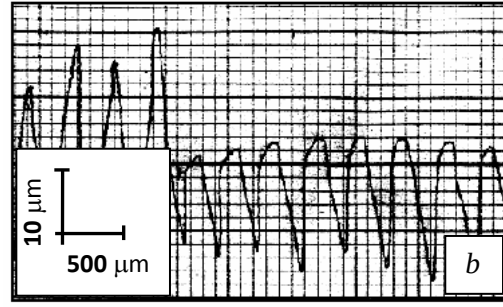
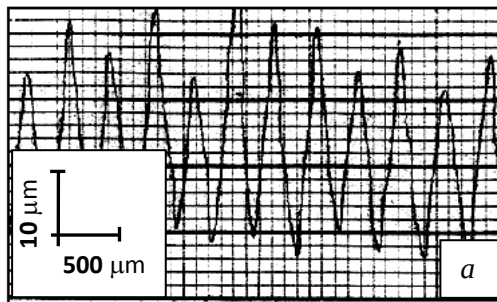


Fig. 1. Fragments of profilograms of a slab surface near the boundary of its contact with a cylinder end before (a) and after the interaction (b).

where h is the height of a microroughness after a contact interaction, H is the initial height of the microroughness, and Δh is the irreversible change in the microroughness height as a result of the contact interaction. In accordance with (21), the formula for determining the relative change in the contrast of the carrying fringes in the speckle photography method takes the form

$$\frac{\Delta\gamma_S}{\gamma_{oS}} = 2 \frac{\Delta h}{H} - \left(\frac{\Delta h}{H} \right)^2 \quad (25)$$

Figures 2a show holographic interferogram of the slab surface under study recorded as fringes of finite widths after the contact between the cylinder end and the slab at a load of 20 kN. Changes in the intensities of the interference fringes over the central cross sections in these patterns are shown in Figs. 2b. The fringe contrast in the central region of the contact spot (Fig. 2a) is 0.6.

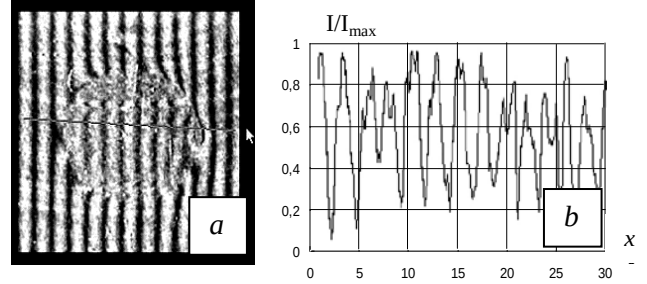


Fig. 2. Holographic interferogram of a slab surface (a) after the contact with a cylinder end and the corresponding distribution of the normalized intensities of the interference fringes in the central cross section of contact zone (b).

Figures 3a show characteristic patterns of Young's fringes obtained as a result of scanning of twice-exposed speckle photographs of the slab surface image (after the cylinder was loaded with a force of 20 kN) at points located in center of the contact zone. The intensity distributions over the central cross section of the diffraction halo are presented in Figs. 3b.

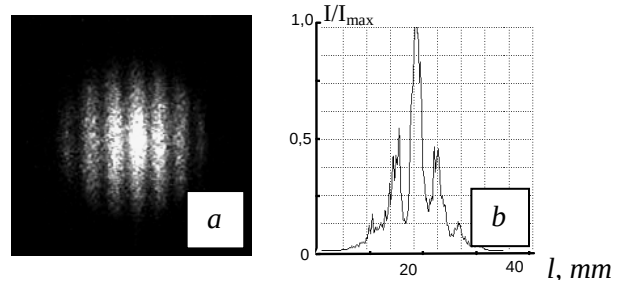


Fig. 3. Young's fringes obtained as a result of scanning of twice-exposed speckle photographs of the slab surface image after the cylinder was loaded with a force of 20 kN (a) and intensity distributions over the central cross section of the diffraction halo (b).

The contrast of Young's fringes beyond the contact zone is $\gamma_o = 0.9$, and, at the center of the contact spot, $\gamma_1 = 0.41$. Similar experimental results were obtained for the contact interaction between the cylinder end and the slab at a load of 30 kN (table).

Tab.1 Experimental data on the relative changes in microrelief heights and the fringe contrast in holographic and speckle interferometry for different contact pressures.

Point no.	P, kN	$\Delta h/H$	$\Delta\gamma_H/\gamma_{oH}$	$\Delta\gamma_S/\gamma_{oS}$	q_{cal} , MPa
1	20	0.31	0.32	0.54	57
2	30	0.48	0.50	0.76	85

4. Conclusion

Substituting the data listed in the table into formulas (24) and (25) showed that the change in the fringe contrast is uniquely related to the relative change in the roughness height and, as a consequence, to the contact-pressure values at the point considered. Hence, the method analyzed in this paper for determining contact pressures during the interaction of objects with rough surfaces, which is based on recording of the change in the contrast of the carrying Young's fringes, does not require that intermediate bodies be introduced into the contact zone and ensures a higher reliability of measurements.

5. Literature

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STRATEGY OF THE COMMERCIAL SIGNAGE

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Anotation: Analyzing subject of this report is the trademark as a individualizing element, image mark and intangible asset for any organization. The author of the publication proves that the management of the trademark is a key aspect in the overall management of modern organizations regardless of the fact that currently it is not a focus of managers. The report suggests separation of an independent functional strategy of trademark management, named as “Strategy of commercial signage”. This strategy creates new opportunities and avoid the clichés of strategies like “red ocean”.

KEY WORD: TRADEMARK, STRATEGY, TACTICS, STRATEGY MAPS, MANAGEMENT

1. Introduction

Strategic management is an art which can be a mile stone for the organization and can overcome time only if there is freedom of thought and expression. The author suggests new approach in this article, in the light of the trademark, with a point beyond of the limited stereotypes of the “red ocean”. The beginning is connected with differentiation of new basic type functional strategy with subject trademark, relating to the differentiation strategy¹. [Galizova-Dimitrova, M, Strategies for management of the trademark – Veliko Tarnovo, 2014]

2. Problem discussion

The management of the trademark is undoubtedly a key aspect of the whole management of the organization. The type, the scale and the sector of functionality are of no matter; the trademark is always applicable as identifier, carrier of the brand, immaterial asset. *The trademark is both in the basis and on the top of the organization (it can be use as company name). The trademark is typical integrative mean in the organization, which value creates and develops, this gradation sets the speed of the whole organization.* David Northon and Robert Kaplan integrated the principle of strategic simultaneousness, which is used for the creation of the value of the organization of immaterial assets, in the core of this principle stays the trademark. She is part of all of their strategy maps and the trademark is deeply analyzed from economic point of view. The conclusion is that the trademark is valuable internal regulator of the organization, mean of communication with the clients and the partners as indicator of the sensor’s mnemonics, it need an individual program of management and it the same time it is the core of corporative strategy. (check fig. 1 Trademark – integrative instrument between internal and external environment of the organization).

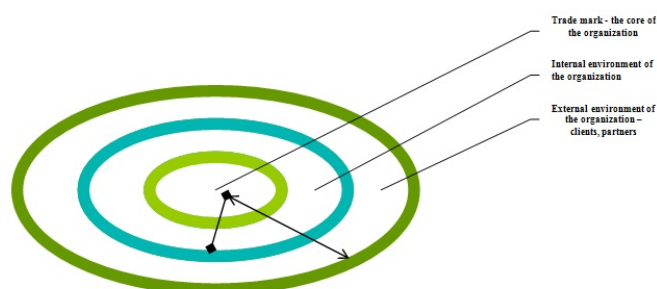


fig. 1 Trademark – integrative instrument between internal and external environment of the organization)

¹ The science of strategic management has different scientific positions about the diversification of the strategies, the author of this article adopts the thesis of Kiril Todorov, which shows that the strategies on different management levels are: corporate strategy, business strategy and functional strategies [Todorov, K. Strategic management in small and medium enterprises, volume I – S, 2001, pages 159-163]. The last strategies are interpret in different way in scientific literature, but in all analyzes the trademark is perceive as element of marketing

Norton and Kaplan identifies the reliable trademark for the needs of their economics research as one of the seven foundation materials of the strategy (Robert S. Kaplan, David P. Norton, Strategy Maps. Converting Intangible Assets into Tangible Outcomes, S., p. 217). The management of the trademark gets together all separate elements of the organization in its internal environment and present the organization in her full glory into the external environment. The cross point between the internal and external environment is the trademark. Apart from its balancing function, the trademark cam lead to some cataclysms if is not manage properly. Taking into account the above each step of the decision of registration of a trademark – type, territory, affects directly the whole activity of the organization. The reason is in its spectrum – different resources (human, material); it develop communicational channels(in the organization and between it and the external environment); it has representative function and with time it starts to build reputation and at the same time it is source of income. Its proper management which starts with the process of creation, pre-registration, registration procedure, contains of potential incomes. On the opposite, the not proper management will lead to losses. From this aspect the trademark is risky asset but nowadays it is key point and indicator of successful business.

The author agrees with Marin Paunov’s point of view about the internal separation of the functional strategies **but he adds the trademark strategy which contains rules for management the trademark**, represented on figure 2. Type of strategies in the organisation. (Paunov, M. Business strategies – S., 2012, pages 162-172. We will use wider concept because in order to have more undoubted success we consider for reasonable to use the relations of the trademark with, domain name, which are used as identification, too and the company transfer the company into different level including virtual one.

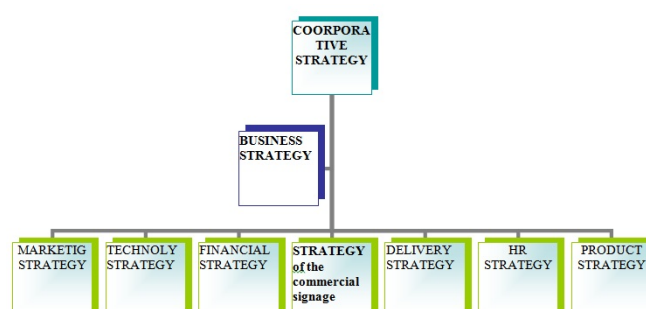


fig. 2. Type of strategies in the organisation

The author consider for reasonable to state the commercial signage strategy as functional because its capability. Steadily this type of strategies are considered as supporting and focused only on one concrete significant aspect from the organizational activity. They are basic, on their basis the business and corporate strategies are developed. There is chance the process to be from down to up - from functional to corporative strategies and back. The different levels of the strategy tree are in coordination and subordination in

order the organization to function as one whole. The function of the trademark is really significant in the process of formulation of the mission and vision because it has really valuable characteristics. It helps the positioning of the organization and creates and supports its reputation. In this content, we should take into account this element in the beginning when we formulate the aim of the organization, if the process starts from the top with creation of the corporate strategy. The strategy of the trademark contains different aspects – managerial, jurisdictional and others. The brand in particular is seen as a mean of competitive power and it is stated for external competitive advantage. (Georgiev, R. Strategies and competitive power – S., 2013, page 27). We can name it strategy of trademark because of the relation between the trademark – company – domain or we can use the wider term strategies of business identifiers which includes a lot of subjects of industrial property, including the ones in the virtual field. The internal and external environment is not only the one of social interaction, it includes the powerful virtual environment, too. We need to take into consideration the technologies presence in the management and virtual markets which determines new type of strategy. The development of new models of trademark strategies as functional strategy through analyze of the laws and cases theory of each country will determine the development of new type of strategy which contains the knowledge, the cultural identity and the psychology of human factor.

In Bulgaria we use the common rules which are kind of axioms without taking into account the factors of the external environment – the law regulation, the court cases, cultural specifics and other. ***The author considers that there is necessity of change of the point of view and focus on the trademark. The first step is its independent analysis from functional aspect which will reflect on to the business and the corporate strategies seen in their ascending gradation. The innovation approach in changing the basis of the pyramid of the strategy will lead to quality changes in the top – in the stating of the aims of the company. (the formulating of the politics, the vision and the mission of the company)².***

3. Conclusion

The idea of introduction of new function in the management through the trademark has been considered during 1931 - its authors are Procter and Gamble – the founders of the company with the same name. IT is not formulated in its basics and it didn't find support in the marketing field. It has been monopolize by the marketers and nowadays it is seen as a small, not significant part of bigger functional marketing strategy. We consider it as a subject with its own existence and the managers should change their points of view and management approach taking it into account. The trademark has wide developed range of laws and court case and it is a synonym of today's manufactures and not only. It shouldn't stay in shadows when formulating the whole strategy of management because it affects the whole vision of the organization including the formulation of the company reputation. In this aspect we want to point out one more proof of the necessity of formulating function theory with a core – the trademark.

² Please look at the definitions of the terms which are provided by Kiril Tododrov. - Todorov, K. Quotation, 36-37.

CONCEPT FOR THE DEVELOPMENT OF A NEW TYPE CARBON CATALYST DESIGNED FOR PROTECTION AGAINST VAPOURS OF HIGHLY TOXIC SUBSTANCES

КОНЦЕПЦИЯ ЗА РАЗВИТИЕТО НА НОВ ТИП ВЪГЛЕН КАТАЛИЗАТОР ПРЕДНАЗНАЧЕН ЗА ЗАЩИТА ОТ ПАРИТЕ НА ВИСОКОТОКСИЧНИ ВЕЩЕСТВА

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ABSTRACT: A concept is presented for the development of a carbon catalyst for protection from vapours of highly toxic substances, different from the ASC Whetlarite type of impregnated Cu/Cr/Ag carbons, based on the analysis of the disadvantages of the breathing filters of contemporary gas masks. It is concluded that promising carbon catalysts will possess higher stability with respect to aging and better protective properties in regard to a considerable number of industrial toxic compounds.

KEY WORDS: PROTECTION AGAINST CWA, ASC WHETLARITE TYPE CARBON, IMPREGNATED ACTIVATED CARBON, DEACTIVATION OF ASC WHETLARITE TYPE CARBON, CARCINOGENIC Cr⁶⁺

The experience gained during World War I has shown that although activated carbon has the capacity to remove the vapors of the majority of chemical warfare agents by means of physisorption, its application in gas mask filters requires modification due to two reasons:

- activated carbon was found to be ineffective when used against highly volatile non-persistent chemical warfare agents such as hydrogen cyanide, cyanogen chloride, phosgene, arsine and phosphine;
- the disposal of used activated carbon is problematic, as handling such contaminated material becomes difficult and raises concerns over safety.

Furthermore, there is a possibility of cross-contamination due to desorption upon its improper disposal after use [1].

At the end of World War I, as a solution to these problems, was initiated addition of chemical sorbent (typically soda-lime) to the activated carbon in gas mask filters. A typical example of this technology is the American M1 Model gas mask ("1919 Model") [2]. The combination of activated carbon and chemical sorbent increases the protection capacity of gas mask canisters against highly volatile acid gases (Table 1), which is due not only to physisorption that takes place, but also to removal from air and destruction of persistent agents by means of chemisorption. That principle is still in use in modern military gas masks.

In this way, gases which the activated carbon does not hold firmly by physisorption and which are gradually given off by its surface, are caught by soda-lime (a mixture that consists of hydrated lime, cement, kieselguhr, sodium hydroxide and water in various proportions [2]) via chemical reaction (i.e. chemisorption, as mentioned above).

Table 1. Types of chemical warfare agents (CWA) and corresponding materials for their neutralization used in M1 Model ("1919 Model") gas mask canisters.

Type of CWA	Neutralizing materials
Bromobenzyl cyanide	Activated carbon
Chloropicrin	Activated carbon
Mustard gas	Activated carbon
Chlorine	Activated carbon + soda-lime mixtures
Phosgene	Activated carbon + soda-lime mixtures
Diphosgene	Activated carbon + soda-lime mixtures
Hydrogen cyanide	Activated carbon + soda-lime mixtures
Lewisite	Activated carbon + soda-lime mixtures

As a result from the considerable research on modification of activated carbon materials used in gas masks (mainly with inorganic phases) conducted during the period between the two World Wars and especially after the World War II, the sorption capacity of the manufactured carbon materials against the non-persistent chemical warfare agents (given in Table 1) was substantially increased.

Table 2 illustrates different compositions for impregnation of activated carbon in gas masks for protection against non-persistent chemical warfare agents, which have been used by the armies of different countries during World War II.

Table 2. Types of activated carbon impregnants used in gas mask canisters according to [3].

Type of impregnant	Form of application	Functions
Copper	Cu, CuO, Cu ₂ O, CuS	Reactant: $\text{Cu}_2\text{O} + 2\text{HCN} \rightarrow \text{H}_2\text{O} + 2\text{CuCN}$ $\text{CuO} + \text{COCl}_2 \rightarrow \text{CO}_2 + \text{CuCl}_2$
Zinc	ZnO, Na ₂ ZnO ₂	Catalyst: $2\text{AsH}_3 + 3\text{O}_2 \rightarrow \text{As}_2\text{O}_3 + 3\text{H}_2\text{O}$ Reactant: $\text{ZnO} + 2\text{HCN} \rightarrow \text{Zn(CN)}_2 + \text{H}_2\text{O}$ $\text{ZnO} + \text{COCl}_2 \rightarrow \text{ZnCl}_2 + \text{CO}_2$
Silver	Ag, Ag ₂ O	Catalyst: $2\text{AsH}_3 + 3\text{O}_2 \rightarrow \text{As}_2\text{O}_3 + 3\text{H}_2\text{O}$
Pyridine	C ₅ H ₅ N	Reactant: $\text{C}_5\text{H}_5\text{N} + \text{ClCN} + \text{H}_2\text{O} \rightarrow \text{CHOCH=CHCH=CHNHCN} + \text{HCl}$

The most successful technology for the preparation of activated carbon for gas masks, which is still in use today, is the so called (in the USA) "whetlerization" process, named after two of its originators – J.C. Whetzel and E.W. Fuller. The essence of this process is the consecutive immersing of activated carbon in appropriate mixtures of impregnants, followed by heat treatment. The carbon materials manufactured by this method are called ASC Whetlarite. In the initial period the US whetlerization process consists of immersing activated carbon in ammoniacal copper carbonate solution, draining off the excess liquid and drying the carbon granules at a temperature sufficient to expel substantially all the ammonia from the granules. Analogous process was developed in Germany, which is done by adding aqueous solution of sodium zincate over the activated carbon material.

In the period after World War II, the composition of active additives for ASC Whetlarite type of carbon materials is supplemented with Cr⁶⁺ and so the active oxide phase of the gas

mask carbon material consists of Cu-, Cr- and Ag-compounds (with or without organic additives).

The ASC Whetlerite type of carbon materials became first choice solution in terms of providing individual and collective protection for the main armies from the second half of 20th century up to now.

The manufacturers of this type of impregnated carbon materials use typically the same components in the production process, although their ratio may vary among different producers. Overall, the Cu-Cr-Ag phase combined with appropriate adsorption and texture parameters of the activated carbon support ensures simultaneous neutralization of practically all types of chemical warfare agents by means of physisorption, catalytic sorption and chemisorption.

The ASC Whetlerite carbon materials are also called activated carbon catalysts based on their catalytic sorption function which they perform in the neutralization of CWA.

At present, the research on the mechanism of removal of non-persistent CWA by ASC Whetlerite is focused primarily on the neutralization of cyanogen chloride (ClCN, an instant break through gas-mask canister's CWA) and hydrogen cyanide (HCN), because of its wide application as a semimanufacture product and feedstock for various industrial productions.

The importance of the active additives for ASC Whetlerite for the removal of phosgene (COCl₂) is not significant, assuming the fact that canister's carbon material catalyses considerably the decomposition of COCl₂, especially in the presence of moisture.

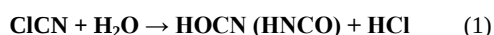
Arsine (AsH₃) and phosphine (PH₃) are presently not used as CWA and regarding organofluorine compounds, the importance of active additives is not fully clarified.

The destructive removing of ClCN by ASC Whetlerite is a complex process, which, depending on Cu:Cr ratio, the presence of moisture and temperature, is carried out by catalytic sorption, chemisorption (to a less extent) and physisorption (at lower temperatures, ≤ 253 K).

The dominating catalytic sorption in the above mentioned case is not expressed as a strictly defined process, but is an aggregate of parallel processes which result in the irreversible poisoning of the active additives in ASC Whetlerite by the reaction products or intermediate compounds.

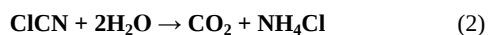
Among catalytic reactions, the two-stage hydrolysis process plays the role of a limiting factor.

During the first stage, the hydrolysis of ClCN is catalyzed by Cu²⁺ to a mixture of cyanic acid (in equilibrium with isocyanic acid) and HCl:

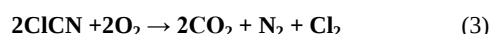


It has been proven that if the active additives for ASC Whetlerite contain only Cu²⁺, the chemical reaction ends at the first stage.

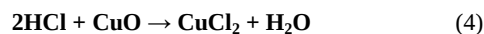
The second stage is ensured by the presence of Cr⁶⁺. The reaction is catalyzed by HCrO₄⁻ to the separation of CO₂ and NH₃:



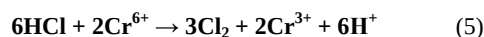
The parallel catalytic oxidation of ClCN is also possible:



Part of the HCl separated during the first stage of the reaction (hydrolysis) reacts with NH₃, while the greater amount of HCl combines with CuO, poisoning it irreversibly:



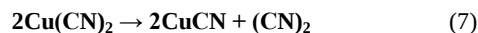
After the depletion of CuO the hydrochloric acid reacts with the chromates (i.e. reduces Cr⁶⁺ to Cr³⁺):



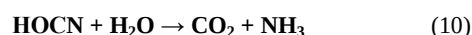
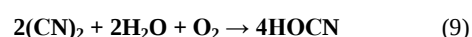
Despite of the considerable research that has been conducted, the actual mechanism of HCN neutralization by ASC Whetlerite carbon is not fully known. At present, it is accepted that Cu²⁺ are the most important ingredient of the active additives for ASC Whetlerite for this purpose. This is due to the significant importance of the reaction between CuO from the additive phase and HCN:



Copper cyanide (Cu(CN)₂) produced in this reaction is an unstable compound and decomposes quickly by the following reaction:



The latter reaction yields cyanogen (dicyan, (CN)₂) which is a highly toxic gaseous substance that can be neutralized by the following reactions:



According to [4] around 15 – 20 % of HCN are neutralized by ASC Whetlerite (depending on Cu/Cr ratio) at the expense of the catalytic oxidation. The reaction is catalyzed by Cu²⁺:



The obtained cyanic acid decomposes typically to CO₂ and NH₃ under the action of Cr⁶⁺ (Reaction 10).

It can be concluded that the formation of (CN)₂ and HOCN as a result from chemical reaction (6) and the catalytic oxidation of HCN (Reaction 11) are due to Cu²⁺ in the composition of ASC Whetlerite impregnated carbon, while Cr⁶⁺ ions take part in the catalytic decomposition of (CN)₂ (Reaction 8) and HOCN (Reaction 10). Nevertheless, the removal of copper from the impregnation compositions for activated carbon is unacceptable, as CuO ensures or participates in the neutralization of the vapors of other non-persistent chemical warfare agents such as phosgene, arsine and chlorine.

Despite of their proven high efficiency in respect to protection against highly volatile non-persistent chemical warfare agents, the ASC Whetlerite type of impregnated carbon materials containing Cr⁶⁺ are regarded by the specialists (for example, from the US Environmental Protection Agency) as non-perspective because of the following reasons:

- some forms of Cr⁶⁺ are carcinogenic [5] and pose risk to the production staff and army personnel, which use the respective gas masks and collective protection equipment;
- the problems associated with the disposal of this type of impregnated carbon materials after the end of their expiration date (defined by the manufacturer);
- the irreversible deactivation during use and storage of ASC Whetlerite with increased pre-adsorbed moisture content [4, 6, 9], which is connected to reduction of Cr⁶⁺ to Cr³⁺ and strong decrease of the sorption capacity of carbon materials towards ClCN.

The above mentioned problems dictate the need for creation of a new generation of impregnated active carbon materials for gas mask protection against the vapors of airborne non-persistent chemical warfare agents and some industrial poisonous substances [10]. The composition of the active additives (the active phase) has to ensure:

- high efficiency, no less than that of ASC Whetlerite carbon materials;

- increased aging stability during storage and exploitation;
- composition of the active phase containing no (or minimal amounts of) Cr^{6+} and not allowing (or limiting to a maximum) the formation of side products (like cyanogen) during use;
- increased protection against the vapors of some of the most common poisonous substances in case of industrial accidents or fires.

The analysis of the mechanism of neutralizing HCN, ClCN and COCl_2 vapors by the active additives for impregnated carbon materials with different composition of active phases shows that they have to contain copper and to be composed in such a manner that to ensure:

- high reactivity towards HCN by simultaneously not allowing the formation of free cyanogen;
- compatibility of the different impregnation components and their participation in common reactions;
- high level of protection against the other types of non-persistent chemical warfare agents such as ClCN.

An opportunity for accomplishment of the above mentioned recommendations is the reduction of Cr^{6+} content ($< 0.6\%$) and the inclusion of Zn instead. Based on our experience, the impregnated carbon materials of this type (called ASZC) ensure protection against HCN vapors equal to that of the ASC Whetlerite carbon materials, but perform poorer than the latter in terms of cyanogen formation.

The addition of an alkaline component ($2\% \text{K}_2\text{CO}_3$) to the impregnation composition of ASZC materials solves that problem and increases the protection activity of the carbon catalyst towards some industrial poisonous substances. However, adding more than 2% of alkaline component changes the chemistry of neutralization of other poisonous substances and has a negative overall effect.

In this sense the most perspective solution according to [7, 11, 12] is the complete replacement of Cr^{6+} in ASZC with Mo or V. At present, such change of the impregnation composition of carbon catalysts is partially accomplished only by the USA army. Such impregnated carbon material of a new generation, designated as ASZM-T, is developed by Calgon Corp. [10] and since 1992 is being used in type C2A1 gas mask canisters.

The perspective for the development of a new type of gas mask carbon material depends also on whether the new technology for application of the precursor solutions and the following thermal treatment of the impregnated carbon materials will distinguish significantly or not from the ASC Whetlerite carbon materials production.

Solution of the problem with ensuring protection against ClCN vapors is achieved by adding 3.5% mass % triethylenediamine (TEDA) to the active additives of ASZM carbon materials. The aging is being reduced by adding TEDA or pyridine.

The additional and mandatory inclusion of TEDA (pyridine) or K_2CO_3 in the impregnation compositions for the new type of carbon materials demands higher requirements towards the texture parameters of the base carbon materials. The latter can be summarized to the following:

- Specific surface area (measured by the BET method) of the base activated carbon materials no less than $1200 \text{ m}^2/\text{g}$;
- Volume of micropores (V_M) no less than $0.7 \text{ cm}^3/\text{g}$;
- Ratio between the volume of micropores and volume of mesopores less than that for ASC Whetlerite carbon materials, at the expense of the volume of supermicropores.

Conclusion

1. The perspective new carbon catalysts will be based on impregnation compositions different from those for the preparation of ASC Whetlerite materials.
2. The new type of carbon catalysts will have no or significantly reduced ($< 0.6\%$) Cr^{6+} content. Instead they will contain Cu, Zn, Mo (V) and also tertiary amines (mostly TEDA) which will improve their anti-aging properties and broaden the area of application against vapors of industrial poisonous substances.
3. The requirements for the texture parameters of the base activated carbon materials are raised, which will increase the final price of the product.

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ANALYTICAL ANALYSIS OF THE INVERSE STABILITY PROBLEM FOR SOME CLASSES OF NON-LINEAR DYNAMICAL SYSTEMS WITH A SMALL UNCERTAIN PARAMETER

АНАЛИЗ ОБРАТНОЙ ЗАДАЧИ УСТОЙЧИВОСТИ ДЛЯ НЕКОТОРЫХ КЛАССОВ НЕЛИНЕЙНЫХ ДИНАМИЧЕСКИХ СИСТЕМ С МАЛЫМ НЕОПРЕДЕЛЕННЫМ ПАРАМЕТРОМ

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Abstract: In this paper we propose a method of solving inverse stability problem for some classes of non-linear dynamical systems with a small uncertain parameter. The method is based on T. Kato's perturbation theory of linear operators. We illustrate our method by solving inverse stability problem in the situation of monomerization reaction inside the cascade of chemical reactors.

KEYWORDS: LOW UNCERTAINTY OF PARAMETERS, PERTURBATION THEORY, SOLUTION IN A BOUNDARY LAYER

1. Introduction

This paper presents an analytical solution of the inverse problem of stability in the cascade process of monomerization when three chemical stirred tank reactors are used under the conditions of uncertainty of some of the reactor's parameter. The decision is based on the perturbation theory of linear operators of Kato-Rellich [1]. The process is carried out by distilling monomerization reagent from one reactor to another. The necessary cooling of the substance is carried out by the coolant in the reactor jacket. The scheme of this stage [2] is shown in Figure 1.

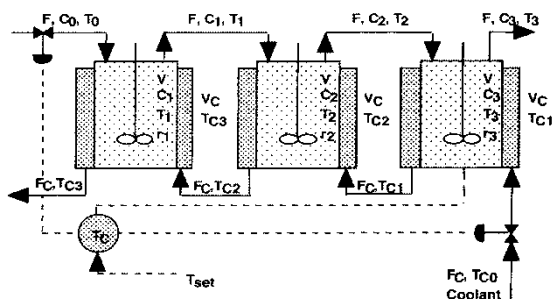


Fig.1. Scheme of the cascade of chemical reactors

The equations describing this process are as follows [2, 3, 4]:

$$\begin{aligned} V \frac{dC_1}{dt} &= F(C_0 - C_1) - Vk(T_1)C_1, \\ \rho c_p V \frac{dT_1}{dt} &= F\rho c_p(T_0 - T_1) + Vk(T_1)C_1\Delta H - \\ &\quad - K_t A(T_1 - T_{c3}), \\ \rho c_p c_{pc} V_c \frac{dT_{c3}}{dt} &= F_c \rho c_p c_{pc}(T_{c2} - T_{c3}) + K_t A(T_1 - T_{c3}), \\ V \frac{dC_2}{dt} &= F(C_1 - C_2) - Vk(T_2)C_2, \\ \rho c_p V \frac{dT_2}{dt} &= F\rho c_p(T_1 - T_2) + Vk(T_2)C_2\Delta H - K_t A(T_2 - T_{c2}), \\ \rho c_p c_{pc} V_c \frac{dT_{c2}}{dt} &= F_c \rho c_p c_{pc}(T_{c1} - T_{c2}) + K_t A(T_2 - T_{c2}), \\ V \frac{dC_3}{dt} &= F(C_2 - C_3) - Vk(T_3)C_3, \\ \rho c_p V \frac{dT_3}{dt} &= F\rho c_p(T_2 - T_3) + Vk(T_3)C_3\Delta H - K_t A(T_3 - T_{c1}), \\ \rho c_p c_{pc} V_c \frac{dT_{c1}}{dt} &= F_c \rho c_p c_{pc}(T_{c0} - T_{c1}) + K_t A(T_3 - T_{c1}) \end{aligned} \quad (1)$$

The parameters of the process are given in Table 1 [2, 3, 4].

Table 1. Process parameters

№	Name	Description	Demention
1	A	Surface contact area	m ²
2	C ₀	Initial concentration of the reactant in the first reactor	kmol/m ³

3	C _j	Concentration of the reactant in the j-th reactor	mol/m ³
4	ρ	Density of the reagent	J/kg·K
5	ρ _c	Density of the refrigerant	J/kg·K
6	E	Activation energy	J/ mol
7	F	Flow rate in the reactor	m ³ /s
8	F _c	Flow rate of the refrigerant	m ³ /s
9	R	Gas constant	J/mol·K
10	c _p	Specific heat of a substance	kg/m ³
11	c _{pc}	Specific heat of the refrigerant	kg/m ³
12	T _{cj}	Temperature of the refrigerant in the cooling part of the j-th reactor	K
33	T _{c0}	Initial temperature of the refrigerant	K
14	K _t	Coefficient of thermal conductivity	J/m ² ·s·K
15	V	Volume of the reactor	m ³
16	V _c	Volume of cooling part of the reactor	m ³
17	Z	Multiplier by the Exhibitor	
18	ΔH	Thermal effect of reaction	J/ mol

From a mathematical point of view, the sustainability of monomerization is equivalent to the stability of solutions of the above system (1) of the equation. However, the technical parameters of the system can not be given exactly. The **main objective** is to evaluate the allowable errors of these parameters, which preserve the stability of the process.

2. The perturbation theory of linear operators Kato-Rellich

Let us consider a process that occurs in a dynamic system described by the following differential equation [1, 5]:

$$\dot{x} = Ax + B, \quad (2)$$

where x- state vector, A - matrix of the system parameters (matrix states), B - matrix of absolute terms.

We will use the method of accounting for uncertainty parameters of the system, based on the theory of perturbation of the eigenvalues of component matrices:

$$A = A_0 + \varepsilon A_1 + \varepsilon^2 A_2 + \dots, \quad (3)$$

where we assume that $\varepsilon^2 \ll \varepsilon$. It is known that the eigenvalues of A in this case can be represented as [5]:

$$\lambda_i(\varepsilon) = \lambda_i^{(0)} + \varepsilon \lambda_i^{(1)} + \varepsilon^2 \lambda_i^{(2)} + \dots, \quad (4)$$

where $\lambda_i^{(0)}$ – is j -th eigenvalue A_0 . Right and left eigenvectors corresponding to the eigenvalues $\lambda_j(\varepsilon)$, for which the following equation: $y_j^T(\varepsilon)x_j(\varepsilon) = 1$ holds true, also expanded in power series: $x_j(\varepsilon) = x_j^{(0)} + \varepsilon x_j^{(1)} + \varepsilon^2 x_j^{(2)} + \dots$, $y_j(\varepsilon) = y_j^{(0)} + \varepsilon y_j^{(1)} + \varepsilon^2 y_j^{(2)} + \dots$. And eigenvalues $\lambda_j^{(1)}$ и $\lambda_j^{(2)}$ are calculated as follows:

Step 1. Calculate the eigenvalues λ_j of matrix A_0 .

Step 2: Finding the right and the left normalized eigenvectors A_0 :

$$(A_0 - \lambda_j I)x_j = 0, y_j^T(A_0 - \lambda_j I) = 0, |x_j| = 1, |y_j| = 1.$$

Step 3. The matrix Z_{k0} is constructed: $Z_{k0} = \frac{\prod_{j=1, j \neq k}^s (A_0 - \lambda_j I)}{\prod_{k=1, j \neq k}^s (\lambda_k - \lambda_j)}$,

where s is dimension of A .

Step 4. The matrix E_j is calculated: $E_j = \sum_{k=1, k \neq n}^s \frac{1}{\lambda_j - \lambda_k} Z_{k0}$.

Step 5. Calculated coefficients of the expansion (4) by the formulas: $\lambda_j^{(1)} = y_j^T A_1 x_j$, $\lambda_j^{(2)} = \text{tr}(B E_1 A_2 Z_{10})$.

In this task we assume that $\varepsilon^3 \ll \varepsilon^2$. Therefore, in the above formula (4) it is sufficient to consider the first three terms.

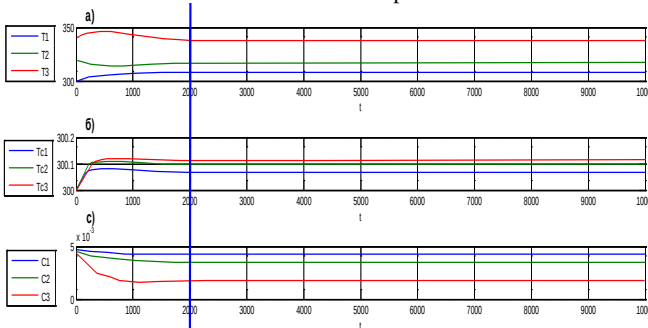
As a criterion for the stability of the system we will use the root criterion, that is, the permissible range of the parameter ε , which is characterized by a system of inequalities of the form for sufficiently small α :

$$\lambda_j(\varepsilon) < -\alpha^2, \quad (5)$$

Solution of the inequality (5) is the intersection of the intervals that are solutions of each inequality. It is obvious that the intersection is not empty, due to the fact since the solution of each inequality will contain zero.

3. Reaching the main objective

Perturbation operators theory developed by Kato, refers to linear operators in function spaces, and the system of equations (1) is non-linear. However, the system (1) can be linearized. Indeed, the experiment [2,3] (Figure 1) shows that the dynamics of changes in the main characteristics of the system admits a linearization, from some point of time from the beginning of the process, and this initial period of time is small relative to the total process time. Thus, during the initial period of time, as it is so small, it is possible to seek the solution of the system by expanding in the time series, and the remaining slot to linearize in the usual manner. At the same time as the initial value of the interval being we linearized site can take the final value of the initial period.



1. a) The plot of a change of a temperature; b) the plot of the change of the temperature of the coolant; c) the graph of the concentration change of the substance

3.1. Constructing an analytical solution of the system at the initial time interval

To unify the system (1) we introduce the following notation:

$C_i = X_i$, $T_i = X_{i+3}$, $T_{ci} = X_{i+6}$, $i = 1, 2, 3$. Then the system of equations for the first reactor takes the following form (the other equations will be similar):

$$\begin{aligned} \frac{dX_1}{dt} &= \frac{F(C_0 - X_1)}{V} - Z \exp\left(\frac{-E}{RX_4}\right) X_1, \\ \frac{dX_4}{dt} &= \frac{F(T_0 - X_4)}{V} + \frac{ZX_1 \Delta H}{\rho c_p} e^{\left(\frac{-E}{RX_4}\right)} - \frac{K_t A (X_4 - X_9)}{\rho c_p V}, \\ \frac{dX_9}{dt} &= \frac{F(X_8 - X_9)}{V_c} + \frac{K_t A (X_4 - X_9)}{\rho c_p V_c}. \end{aligned} \quad (7)$$

Denote $t = T\tau$, where T – the time course of the whole process, and $X_j = \bar{X}_j x_j$, $j = 1, 2, \dots, 9$. Note, that x_j и τ – dimensionless quantities and $\tau \ll 1$. Then the system describing the dynamics of the process in the first reactor takes the form (the other equations will take the same form):

$$\begin{aligned} \frac{dx_1}{d\tau} &= \frac{FTC_0}{V\bar{X}_1} - \frac{FT}{V} x_1 - ZT e^{\left(\frac{-E}{R\bar{X}_4 x_4}\right)} x_1, \\ \frac{dx_4}{d\tau} &= \frac{FTT_0}{V\bar{X}_4} - \frac{FT}{V} x_4 + \frac{ZT\bar{X}_1 x_1 \Delta H}{\rho c_p \bar{X}_4} e^{\left(\frac{-E}{R\bar{X}_4 x_4}\right)} + \frac{K_t AT (x_4 - \frac{\bar{X}_9}{\bar{X}_4} x_9)}{\rho c_p V}, \\ \frac{dx_9}{d\tau} &= \frac{F_c T \left(\frac{T_c}{\bar{X}_9} - x_9\right)}{V_c} + \frac{K_t AT \left(\frac{\bar{X}_4}{\bar{X}_9} x_4 - x_9\right)}{\rho c_p V_c}. \end{aligned}$$

We seek a solution of the system on a small initial period of time as a power series in the small parameter τ : $x_j(\tau) = C_0^j + C_1^j \tau + C_2^j \tau^2 + \dots$, where C_0^j are known and the initial values of parameters of the input vector. The expression $e^{\left(\frac{-E}{R\bar{X}_4 x_4}\right)}$ is expanded in a series

$$\begin{aligned} \text{as a function of the } \tau: \quad e^{\left(\frac{-E}{R\bar{X}_4 x_4}\right)} &= e^{\left(\frac{-E}{R\bar{X}_4 C_0^4}\right)} + \frac{e^{\left(\frac{-E}{R\bar{X}_4 C_0^4}\right)} EC_1^4}{R\bar{X}_4 (C_0^4)^2} \tau + \\ &+ \frac{1}{2} \frac{e^{\left(\frac{-E}{R\bar{X}_4 C_0^4}\right)} E(2R\bar{X}_4 (C_0^4)^2 C_2^4 - 2R\bar{X}_4 C_0^4 (C_1^4)^2 + E(C_1^4)^2)}{(R\bar{X}_4 (C_0^4)^2)^2} \tau^2 + o(\tau^3). \end{aligned}$$

Representation of the solution of the system in the form of a power series in the variable τ and its further substitution in the system of equations gives, by equating the coefficients of corresponding powers of τ , a recurrent system of equations for the coefficients of the expansion of the solution. Here is a small piece of this scheme:

$$\begin{aligned} C_1^1 &= \frac{FTC_0}{V\bar{X}_1} - \frac{FTC_0^1}{V} - ZT e^{\left(\frac{-E}{R\bar{X}_4 C_0^4}\right)} C_0^1, \\ C_1^4 &= \frac{FTC_0}{V\bar{X}_4} - \frac{FTC_0^4}{V} - \frac{ZT\Delta H}{\rho c_p} e^{\left(\frac{-E}{R\bar{X}_4 C_0^4}\right)} C_0^1 - \frac{K_t AT (C_0^4 - C_0^9 \frac{\bar{X}_9}{\bar{X}_4})}{\rho c_p V}, \\ C_2^1 &= \frac{1}{2} \left(-ZT e^{\left(\frac{-E}{R\bar{X}_4 C_0^4}\right)} C_1^1 - \frac{ZT e^{\left(\frac{-E}{R\bar{X}_4 C_0^4}\right)} EC_1^4 C_0^1}{R\bar{X}_4 (C_0^4)^2} - \frac{FTC_1^1}{V} \right). \end{aligned}$$

So it's clear that all the coefficients are calculated consistently.

3.2. Linearization of the system of differential equations of the dynamics of chemical reactors

In the previous section solution of the system at the initial time interval was constructed. Now we construct a solution of (1) in the remaining time interval by its linearization. Note that the solution obtained in the above initial time interval at the end of this interval is the vector of initial values for the remaining time interval.

Represent x_j as follows $x_j = X_j^0(1 + y_j)$, $j = 1, 2, \dots, 9$, where y_j – small quantity, which allows to neglect the terms containing the second order y_j . The main issue arises when converting linearization terms of the form e^{x_j} . For this we use the Taylor

formula:

$$e^{-\frac{c}{x_j}} = e^{-\frac{c}{x_j^{(0)}(1+y_j)}} = e^{-\frac{c}{x_j^{(0)}}} + e^{-\frac{c}{x_j^{(0)}}} \left(\frac{c}{x_j^{(0)}(1+y_j)} \right)'_{x_j=0} \cdot x_j + O(x_j^2).$$

Neglecting the second order x_j^2 , we obtain approximately: $e^{-\frac{c}{x_j}} = e^{-\frac{c}{x_j^{(0)}(1+y_j)}} = e^{-\frac{c}{x_j^{(0)}}} + e^{-\frac{c}{x_j^{(0)}}} \cdot \frac{c}{x_j^{(0)}} \cdot x_j$. Thus, the system of equations for the first reactor takes the form:

$$\begin{aligned} \frac{dy_1}{d\tau} &= \xi_{11}y_1 + \xi_{14}y_4 + b_1 \\ \frac{dy_4}{d\tau} &= \xi_{41}y_1 + \xi_{44}y_4 + \xi_{49}y_9 + b_4, \end{aligned} \quad (8)$$

$$\begin{aligned} \text{where } \xi_{11} &= \left(-\beta e^{-\frac{c}{x_4^{(0)}}} - \alpha \right) X_1^{(0)}, \xi_{14} = \beta \frac{X_1^{(0)}}{X_4^{(0)}} e^{-\frac{c}{x_4^{(0)}}}, \xi_{41} = \\ &= \frac{\beta_H X_1^{(0)}}{\delta} e^{-\frac{c}{x_4^{(0)}}}, \xi_{44} = X_4^{(0)} \left(-\alpha - \frac{\gamma}{\varphi} \right) + \beta_H c \frac{X_1^{(0)}}{X_4^{(0)}} e^{-\frac{c}{x_4^{(0)}}}, \xi_{94} = \\ &= \frac{\gamma \rho}{\varphi c} X_4^{(0)}, \xi_{99} = X_9^{(0)} \left(-\alpha_c - \frac{\gamma}{\varphi c} \right), \quad \text{but} \quad b_1 = \left(-\beta e^{-\frac{c}{x_4^{(0)}}} - \right. \\ &\left. \alpha \right) X_1^{(0)}, b_2 = \left(-\alpha - \frac{\gamma}{\varphi} \right) X_4^{(0)} + \frac{\gamma}{\varphi \eta} X_9^{(0)} - X_1^{(0)} \frac{\beta_H}{\delta} e^{-\frac{c}{x_4^{(0)}}} - \\ &\alpha \theta_4, b_3 = \left(X_9^{(0)} + \theta_9 \right) \alpha_c + \frac{\gamma \eta}{\varphi c} X_4^{(0)}. \quad \text{Where} \quad \varphi = \delta V, \varphi_c = \\ &\delta_c V_c, \beta_H = \beta \Delta H, \eta = \frac{X_4^{(0)}}{X_9^{(0)}}, \theta_4 = \frac{T_0}{X_4^{(0)}}, \theta_9 = \frac{T_c}{X_9^{(0)}}, \quad \text{где} \quad \alpha = \frac{FT}{V}, \beta = \\ &= \frac{ZT}{V}, \gamma = K_t AT, \alpha_c = \frac{F_c T}{V_c}, \delta = \rho c_p, \delta_c = \rho c_p c. \end{aligned}$$

So we obtain:

$$A = \begin{pmatrix} \xi_{11} & \xi_{14} & 0 \\ \xi_{41} & \xi_{44} & \xi_{49} \\ 0 & \xi_{94} & \xi_{99} \end{pmatrix}, b = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}, x = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}.$$

4. Uncertainty parameters of the matrix A

Let's suppose that the uncertainty in parameters reflecting the heat of reaction $-\Delta H$.

Suppose, therefore, that $\Delta H^0 = \Delta H(1 + \varepsilon)$, $[\varepsilon] \ll 1$. Then $\beta_H^0 = \beta \Delta H(1 + \varepsilon)$, and, in turn, the matrix parameters ξ_{41} and ξ_{44} take the form:

$$\begin{aligned} \xi_{41} &= \frac{\beta_H^0 X_1^{(0)}}{\delta} e^{-\frac{c}{x_4^{(0)}}} = \frac{\beta \Delta H^0 X_1^{(0)}}{\delta} e^{-\frac{c}{x_4^{(0)}}} = \frac{\beta \Delta H}{\delta} e^{-\frac{c}{x_4^{(0)}}} (1 + \varepsilon) X_1^{(0)} = \\ &= \frac{\beta \Delta H}{\delta} e^{-\frac{c}{x_4^{(0)}}} X_1^{(0)} + \left(\frac{\beta \Delta H}{\delta} e^{-\frac{c}{x_4^{(0)}}} X_1^{(0)} \right) \varepsilon = \xi_{41}^0 + \xi_{41}^1, \\ \xi_{44} &= X_4^{(0)} \left(-\alpha - \frac{\gamma}{\varphi} \right) + \beta_H^0 c \frac{X_1^{(0)}}{X_4^{(0)}} e^{-\frac{c}{x_4^{(0)}}} = X_4^{(0)} \left(-\alpha - \frac{\gamma}{\varphi} \right) + \\ &+ \beta \Delta H^0 c \frac{X_1^{(0)}}{X_4^{(0)}} e^{-\frac{c}{x_4^{(0)}}} = X_4^{(0)} \left(-\alpha - \frac{\gamma}{\varphi} \right) + \beta \Delta H c \frac{X_1^{(0)}}{X_4^{(0)}} e^{-\frac{c}{x_4^{(0)}}} (1 + \varepsilon) = \\ &= X_4^{(0)} \left(-\alpha - \frac{\gamma}{\varphi} \right) + \beta \Delta H c \frac{X_1^{(0)}}{X_4^{(0)}} e^{-\frac{c}{x_4^{(0)}}} + \left(\beta \Delta H c \frac{X_1^{(0)}}{X_4^{(0)}} e^{-\frac{c}{x_4^{(0)}}} \right) \varepsilon = \xi_{44}^0 + \\ &+ \xi_{44}^1. \end{aligned}$$

Thus, we obtain:

$$A = A_0 + \varepsilon A_0 = \begin{pmatrix} \xi_{11} & \xi_{14} & 0 \\ \xi_{41}^0 & \xi_{44}^0 & \xi_{49} \\ 0 & \xi_{94} & \xi_{99} \end{pmatrix} + \varepsilon \begin{pmatrix} 0 & 0 & 0 \\ \xi_{41}^1 & \xi_{44}^1 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

5. Summary

In this paper, we propose a method of analysis of a nonlinear dynamical system, which describes by a standard process of monomerization cascade of chemical substances in the stirred tank reactors, provided that certain parameters of the reactor have undefined values. Namely: 1) an algorithm to obtain an approximate analytical solution of the corresponding system of nonlinear differential equations has been developed; 2) on the basis of the solution a fairly simple algorithm for its numerical implementation has been derived; 3) the corresponding system of differential equations is transformed to a form, which allows you to explicitly take into account the uncertainty of the parameters of the system, and, therefore, to use the methods of perturbation theory of linear operators by Rellich - Kato.

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SIMPLIFIED ANALYSIS OF DISPERSION AND ATTENUATION OF THE BRAGG FIBER

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Abstract: In this article the mechanism of spreading of optical radiation in a Bragg fiber is considered. A mathematical model for analysis of a Bragg fiber viewed as a flat multilayered dielectric structure has been proposed. The method of geometrical optics of description of spreading the light is used. Formulas connecting the clad refractive index with fiber parameters are given. The light attenuation at its refraction in the multilayered clad and chromatic dispersion are calculated, as well as the dielectric loss of the clad material. The dispersion and the width of the waveband of Bragg fibers with different number of layers and low waveguide modes have been compared. Examples of fibers with different coefficient of dielectric material loss are included.

Keywords: BRAGG FIBER, GEOMETRICAL OPTICS, DISPERSION, ATTENUATION

1. Introduction

In the conventional optical fibers, propagation of the light only in the core is caused by the total internal reflection from the clad. This is possible when the effective refractive index of the core is greater than the cladding. The Bragg fiber is one dimensional fiber and is constructed as uniaxial cylindrical layers. The fiber cladding is a dielectric mirror, realized as a multilayer dielectric coverage [2]. This kind of fibers is a part of so called Photonic Crystal Fibers (PCF) or microstructured fibers. The term marks the most of the optical fibers with a complicated clad structure; which often includes one- or two-dimensional periodic structures and has substantial influence on the optical properties of the fiber [3]. PCF decrease significantly the restrictions, caused by the materials and the construction of the conventional optical fibers and allow the characteristics of the fibers as bandwidth, dispersion, nonlinearity, modal area to be controlled more freely [5]

The attenuation of the light in the fiber during transmission to long distances is critical. In the usual fibers, the attenuation is limited by the Rayleigh scattering of the energy of spreading modes. Because of that, when manufacturing, the fibers should use pureness materials with low dielectric losses.

All PCF allow easy changing of dispersion and can compensate the dispersion in the telecommunication fibers. The high attenuation can be overcome by a new design [6].

Cross-sections of different kinds of optical cylindrical PCF are shown in fig. 1. These fibers have different mechanism to keep the light inside the core.

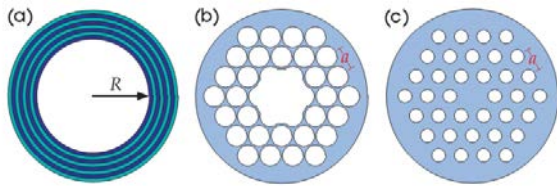


Fig. 1 PCF fibers. (a) Bragg fiber, with a one-dimensional periodic cladding of concentric layer; (b) Two-dimensional periodic structure (a triangular lattice of air holes – “holey fiber”), confining light in a hollow core by a band gap; (c) Holey fiber that confines light in a solid core by index guiding.

Nowadays there is no universal and precise enough method of evaluation of the fiber losses, which allows an optimizing of construction properties (diameter, layers thickness, refractive index of the material) in a given frequency band. Numerical solution of the Maxwell equations is realized in many software systems, but it needs significant computation power. Solution of the system of partial differential equations takes tens of minutes or hours. Despite of some accessible software modules, creating such a completed software tool is not an easy task. The software systems, ready to use, are specialized to analyze a group of similar problems and they are expensive.

Next we will propose an engineering accuracy method for analyzing the light propagation in a multilayer Bragg fiber with a hollow core as a result of tunneling and taking into account the dielectric losses of the fiber clad.

2. Mathematical model

Suppose we have a Bragg optical fiber with M cylindrical layers of cladding. The core refractive index is n_a . A cross-section view of the fiber is presented in Fig. 2.

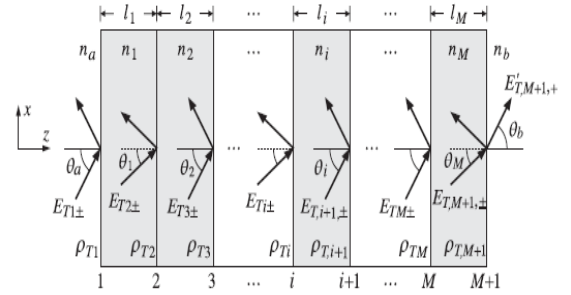


Fig. 2 Oblique incidence in multilayer dielectric structure

Because of central symmetry of the fiber, only half of a longitudinal section is shown. We suppose that the fiber is like a flat multilayer dielectric structure [1]. From the left to the right in the figure are located the core, layer 1, layer 2, layer 3, ..., layer M of the cladding. The symbol n_a marks the core refractive index. n_i is the refractive index of the layer number i . n_b is refractive index of the uppermost layer. The thickness of the layer i is signed as $i=1, 2, 3, \dots, M$. Here $E_{T,k\pm}$, $k=1, 2, \dots, M+1$ marks falling (+) or refracted (-) parts of electrical field at the border of layer k and the layer on the left before it. The leaking field from waveguide is signed as $E'_{T,M+1,+}$. The Snell's law describes the relationship between the angles of incidence and refraction and the refractive indexes of the material at the border surface between every two of all $M+1$ boundary layers:

$$(1) \quad n_a \sin \theta_a = n_i \sin \theta_i = n_b \sin \theta_b,$$

when $i=1, 2, 3, \dots, M$.

We suppose there is no incident field on the right of the structure. Here ρ_{Ti} is a transverse refractive index of surface number i , defined as:

$$(2) \quad \rho_{Ti} = \frac{n_{Ti-1} - n_{Ti}}{n_{Ti-1} + n_{Ti}}, \quad i=1, 2, 3, \dots, M+1,$$

where $n_{T0} = n_a$ and $n_{TM+1} = n_b$. The phase shifting of incident beams, passing through the layer number i is given by $\delta_i = k_0 n_i \cos \theta_i$, where k_0 is the wave number in the free space, $k_0 = \frac{2\pi}{\lambda}$.

In every layer, the transverse refraction factors for *TM* and *TE* polarization are described as:

$$(3) \quad n_{Ti} = \begin{cases} \frac{n_i}{\cos \theta_i}, & \text{TM polarization} \\ n_i, & \text{TE polarization} \end{cases},$$

where $i = a, 1, 2, \dots, M, b$.

The spreading matrix associates the electric field density of the incident with refracted beam recursively:

$$(4) \quad \begin{bmatrix} E_{Ti,+} \\ E_{Ti,-} \end{bmatrix} = \frac{1}{\Gamma_i} \begin{bmatrix} \exp(j\delta_i) & \rho_{Ti} \exp(-j\delta_i) \\ \rho_{Ti} \exp(j\delta_i) & \exp(-j\delta_i) \end{bmatrix} \begin{bmatrix} E_{Ti+1,+} \\ E_{Ti+1,-} \end{bmatrix},$$

where $i=M, M-1, \dots, 1$. Here the refractive factor is $\Gamma_{Ti} = E_{Ti,-}/E_{Ti,+}$ and associates Γ_{Ti+1} with recursion:

$$(5) \quad \Gamma_{Ti} = \frac{\rho_{Ti} + \Gamma_{Ti+1} \exp(-2j\delta_i)}{1 + \rho_{Ti} \Gamma_{Ti+1} \exp(-2j\delta_i)}, \quad i=M, M-1, \dots, 1,$$

where $\Gamma_{T,M+1} = \rho_{T,M+1}$.

A similar association exists between electric and magnetic field on the boundary between 2 layers:

$$(6) \quad \begin{bmatrix} E_{Ti} \\ H_{Ti} \end{bmatrix} = \begin{bmatrix} \cos \delta_i & j\eta_{Ti} \sin \delta_i \\ j\eta_{Ti}^{-1} \sin \delta_i & \cos \delta_i \end{bmatrix} \begin{bmatrix} E_{Ti+1} \\ H_{Ti+1} \end{bmatrix},$$

where $i=M, M-1, \dots, 1$.

In (6) the transverse characteristic impedances are defined as:

$$(7) \quad \eta_T = \begin{cases} \eta \cos \theta & \text{TM polarization} \\ \frac{\eta}{\cos \theta} & \text{TE polarization} \end{cases},$$

where $\eta_{Ti} = \eta_0 / n_{Ti}$. The total power of incident beam P_{in} towards the wave vector direction, its z component and the input power into first layer P_1 for *TE* and *TM* polarizations are given by:

$$(8) \quad P_{in} = \frac{1}{2\eta_a} |E_{in}|^2, \quad P_{in,z} = P_{in} \cos \theta_a,$$

$$\eta_a = \eta_0 / n_a, \quad P_1 = P_{in,z} (1 - |\Gamma_1|^2).$$

The losses of reflection are:

$$(9) \quad \frac{P_1(\lambda)}{P_{in,z}(\lambda)} = 1 - |\Gamma(\lambda)|^2,$$

The normalized attenuation is:

$$(10) \quad B(\lambda) = \frac{P_{in,z}(\lambda) - P_1(\lambda)}{P_{in,z}(\lambda)} = |\Gamma(\lambda)|^2.$$

We discuss a fiber with radius a , core refractive index n_a , cladding refractive index n_1 . The light is spreading when $\sin \theta_a > n_1/n_a$. Fig. 3 shows the trajectory of beams.

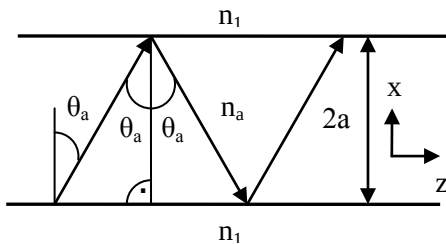


Fig. 3 Meridional beams in the core

The spreading modes of index m have discrete values of the angle θ_a . The transverse resonance condition expresses the phase change for one zigzag of the beam, multiple by 2π :

$$(11) \quad 4ak_0 n_a \cos \theta_a + \varphi = 2m\pi$$

where φ is a phase changed by reflection from the boundary core - cladding. Between two sequential refraction, the path of light beam is $lz = 4a \cdot \tan \theta_a$. If the length of the fiber is equal to L , there are N reflections inside the core, where $N = L/lz$. The losses $B(\lambda)$ in a fiber with length L for *TE* and *TM* polarization are proportional to N :

$$(12) \quad B(\lambda) = N |\Gamma(\lambda)|^2 = \frac{L |\Gamma(\lambda)|^2}{lz}.$$

The reflection factor is $\Gamma(\lambda) = |\Gamma(\lambda)| \exp(\arg(\Gamma(\lambda)))$, and the phase change when the beam passes through the entire fiber is $N \cdot \arg(\Gamma(\lambda))$. The delays of beams with *TE* and *TM* polarization are respectively τ_e and τ_m . They are calculated by an expression [4]:

$$(13) \quad \tau(\lambda) = \frac{\lambda^2}{2\pi \cdot c} \frac{d(\arg(\Gamma(\lambda)))}{d\lambda},$$

where $\Gamma(\lambda)$ is reflection factor for *TE* and *TM* modes.

The chromatic dispersion of the fiber d_{cr} is given by the expressions:

$$(14) \quad d_{cr}(\lambda) = \frac{d\tau(\lambda)}{d\lambda} = \frac{2\tau(\lambda)}{\lambda} - \frac{\lambda^2}{2\pi \cdot c} \cdot \frac{d^2(\arg(\Gamma(\lambda)))}{d\lambda^2}$$

The total attenuation $BN(\lambda)$ along the whole length of the fiber is expressed as a sum of the particular area attenuations $Bi(\lambda)$ in which the reflected beam is signed with integer number $1, 2, 3, \dots, N$, as follows:

$$(15) \quad \begin{aligned} B_N(\lambda) &= B_1(\lambda) \cdot B_2(\lambda) \cdot B_3(\lambda) \dots B_N(\lambda) = \\ B_i^N(\lambda) &= (\Gamma^2(\lambda))^N. \end{aligned}$$

In expression (15) $\Gamma(\lambda)$ are complex refractive coefficients in areas with incident angle θ_a :

$$(16) \quad \Gamma(\lambda) = \alpha + j\beta.$$

The real part α accounts the propagation losses, and the imaginary part β is a phase coefficient. When in the clad there are dielectrical losses, the refractive index n and wave vector k are complex numbers too:

$$(17) \quad n = n' - jn'', \quad k = k' - jk'',$$

The propagating electrical field trough z axis is represented as:

$$(18) \quad \begin{aligned} E(z) &= E_0 \exp(-\Gamma z) = E_0 \exp(-\alpha z) \exp(j\beta z) = \\ &= E_0 \exp(-jkz) = E_0 \exp(-k''z) \exp(-jk'z) = \\ &= E_0 \exp(-k''z) \exp(-j \frac{2\pi n'}{\lambda} z). \end{aligned}$$

The phase coefficient β can be expressed by the real part of the refractive coefficient α and the wave length in free space λ as $\beta = \frac{2\pi n}{\lambda}$. Usually

$$(19) \quad \alpha [dB/km] = 10 \lg(\alpha z).$$

From (17, 18, 19) follows:

$$(20) \quad \alpha = k'' = \frac{2\pi n''}{\lambda}, \quad n'' = \frac{\lambda \alpha}{2\pi}.$$

When dielectrical losses are low, $n'' \approx \tan \delta$.

3. Examples

Let's have a M -layers Bragg fiber with an air core, a core radius $a=62\text{ }\mu\text{m}$; $n_a=1.0$, $n_b=1.5$. The cladding consists of three different materials, each of them having different losses. (H , L , b layers). The thickness of the layers is chosen so as to make a phase difference of 90° for the central wave length $\lambda_0=1500\text{nm}$.

The user enters loss coefficients of the layers α_H , α_L , α_b . After solving the characteristic equation (11) for $m=1$ and doing some calculations according to the above proposed mathematical model, we obtain as a result the refractive coefficients of the multilayer cladding.

Then we calculate the normalized attenuations $B_{te}(\lambda)$ for TE polarization in [dB] for a fiber without deformation.

After that, we obtain the group delay and dispersion. The influence of the losses α [dB/km] of the clad on the attenuation of TE wave is shown in fig. 4.

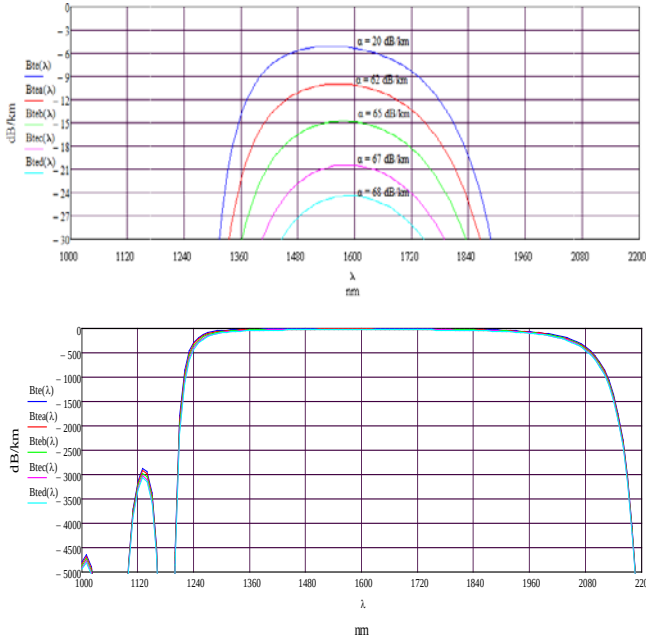


Fig. 4 Attenuation $B_{te}(\lambda)$ when the material has different losses. The upper diagram range is 30 dB; the lower diagram range is 5000 dB

Fig. 5 shows a comparison between attenuations B_{te} of the first TE mode in the Bragg fiber with $M=9$ layers of the cladding and conventional SMF, depending on losses of material α [dB/km], when the wavelength is fixed to $\lambda=1550\text{nm}$.

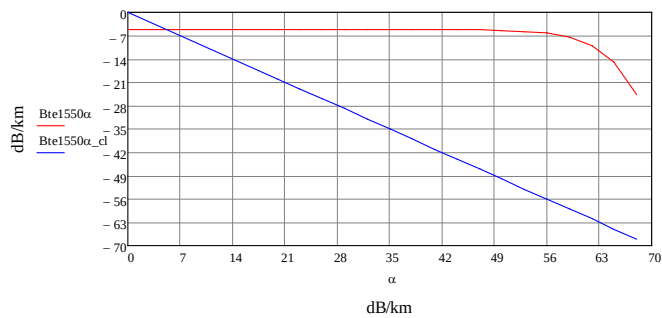


Fig 5 Attenuation of Bragg fiber and SMF when losses of the clad are different

The comparison of the attenuation of the Bragg fiber and conventional SMF shows, that in case of $\alpha < 7\text{dB/km}$ the conventional SMF has lower attenuation per unit length. When losses α rise above 7dB/km , the Bragg fiber can have lower attenuation than SMF.

Fig. 6 shows changing of the attenuation of the fundamental TE mode ($m=1$), in a Bragg fiber with core radius $a=62\text{ }\mu\text{m}$, $\lambda=1550\text{nm}$, as function of losses in material α . Here are some

diagrams of the attenuation $B_{te}(\alpha)$ in a fiber with different number of clad layers ($M=9-21$). The diagram shows, that with increasing of the number of the dielectric clad layers the attenuation of the fibers decreases, this decreasing changing more intensively in fibers containing fewer numbers of layers in the clad, than in fibers containing over 13 layers in the clad. The increasing of α above 50dB/km abruptly increases total attenuation of the fiber. However, even in fibers with 11 layers and losses $\alpha < 68\text{dB/km}$, total attenuation is less than -20dB/km .

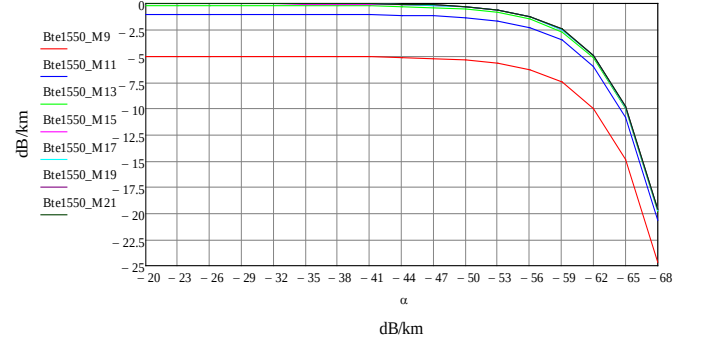


Fig. 6 Attenuation $B_{te}(\alpha)$ in a Bragg fiber with $M=9-21$ cladding layers

Fig. 7 shows shifting of the maximum of the wave characteristic of the Bragg fiber with different numbers of layers $M=9, 11, 13, 15$, when losses of material in cladding α increase. It is shown that this shifting depends more strongly on losses of the material cladding α in fiber with larger numbers of layers in the clad.

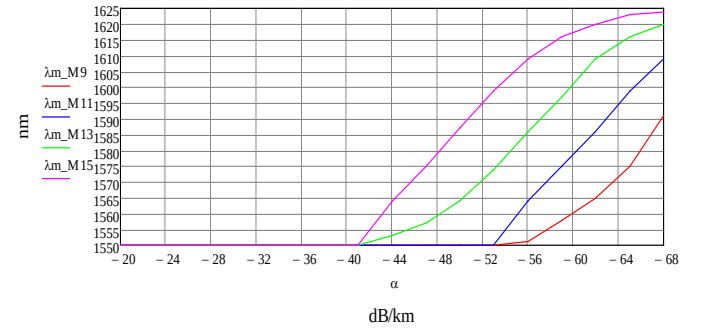


Fig.7 Maximum of the wave characteristic, depending on the losses in a fiber with different number clad layers

Fig. 8 shows the changing of the bandwidth $\Delta\lambda$ [nm] of the wave characteristic $B_{te}(\lambda)$ on level -3dB , depending on the losses of the fiber cladding material α [dB/km] when $M=9, 11, 13, 15$ cladding layers.

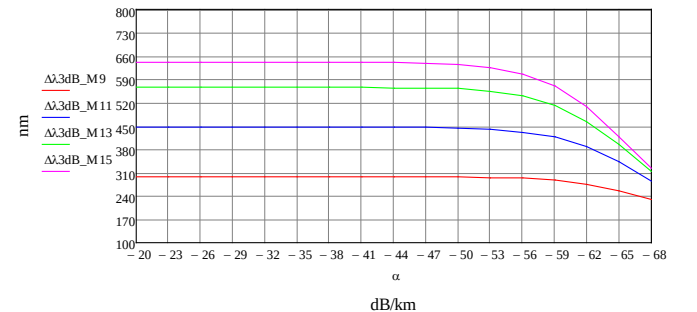


Fig. 8 Changing the bandwidth, depending on losses in a fiber with different number clad layers

The bandwidth $\Delta\lambda$ is narrower in fiber with fewer numbers of layers and decreases when α rises. For example, when $M=9$ layers, and $\alpha=0\text{dB/km}$ the bandwidth is $\Delta\lambda=300\text{nm}$ and when $\alpha=68\text{dB/km}$ the bandwidth decreases to $\Delta\lambda=230\text{nm}$.

Fig. 9 shows the changing of the steepness st_{plus} and st_{minus} of short wave and long wave slopes of the wave characteristic

$Bte(\lambda)$, depending on the losses α [dB/km], the number of clad layers being $M=15$.

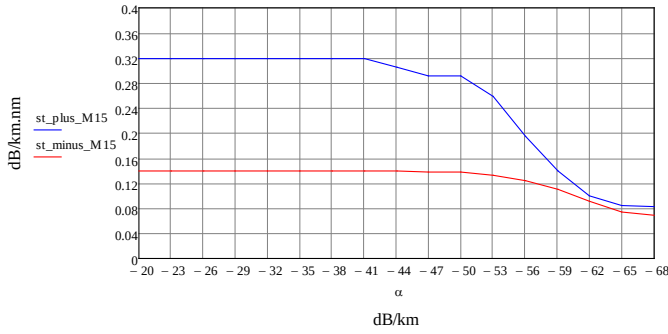


Fig. 9 Slope of the wave characteristic as a function of losses

The studies show that steepness of the slopes of wave characteristics rises when the number of fiber layers rises due to the decreasing of the attenuation and increasing the flatness of the wave characteristic $Bte(\lambda)$ in the bandwidth.

Fig. 10 shows the attenuation $Bte(\lambda=1550nm)$ in the fiber as a function of clad material losses $\alpha=20-68dB/km$. On a common diagram are represented attenuations in fibers with $M=9$ layers and different core radius ($a=10-100\mu m$).

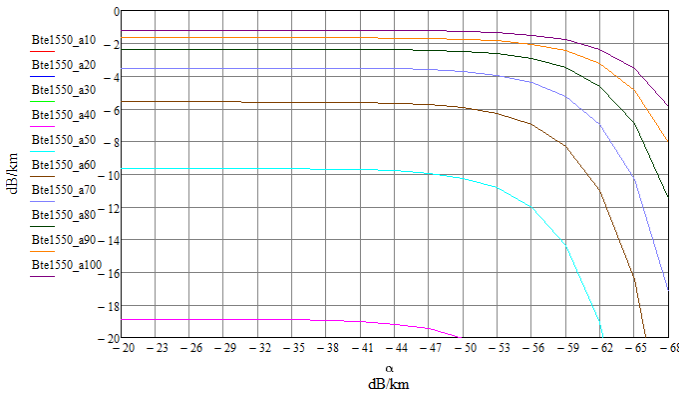


Fig. 10 Attenuation, depending on the losses in a fiber with different core radius

The chart demonstrates the decreasing of attenuation of the Bragg fiber, when the radius of the hollow core increases.

Fig. 11 presents the attenuation of the same fiber as a function of the clad material losses, presented by $tg\delta$ and with different fiber core radius ($a=10-100\mu m$).

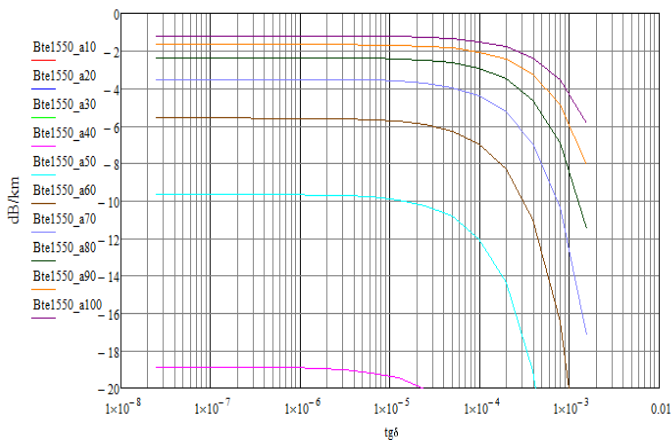


Fig 11 Attenuation of the fiber as a function of clad material losses and core radius

4. Conclusion

The proposed mathematical model and the calculation algorithm allow an approximate analysis of the basic characteristics of Bragg fiber. This method makes it possible for optical fibers with M ($M \leq 21$) clad layers to be analysed. The obtained numerical results show the influence of losses of real dielectric materials over the attenuation of the wave propagation in the Bragg fibers.

The comparison between the attenuation of Bragg fiber with small numbers of layers ($M=9$) and conventional SMF with the same dielectrical losses, α of the material clearly shows that the Bragg fiber has an attenuation greater than the usual SMF, when the losses in the dielectric clad are small ($\alpha < 7dB/km$) due to limited transparency of the cladding. The increasing the losses in the dielectrical cladding ($\alpha > 7dB/km$) makes the Bragg fiber attenuation less than the attenuation in the SMF. In case when $\alpha < 20dB/km$, losses of the dielectric material slightly influence over the attenuation in the fiber. This difference becomes very small when losses exceed $60dB/km$ ($tg\delta > 10^{-4}$). The attenuation increases very fast (by more than $20dB/km$) when $\alpha > 70dB/km$. This means that to manufacture Bragg fibers, it is not necessary to use the complicated technology, to get pure materials, usually used for conventional optical fibers.

Increasing the fiber air core radius decreases the attenuation in the fiber.

The bandwidth decreases relatively slightly when the losses of the material increase. The wave characteristic is asymmetric, its short wave slope being shorter and steeper and the long wave one more gradual and longer. The steepness of the slopes depends on value of the losses. When the losses of clad material increase, the steepness of short wave slope decreases and the steepness of the long wave one increases.

When the dielectric losses increase, the dispersion and the group delay time decrease.

The method of geometrical optics is less accurate than numerical methods of calculations of the field, used in some software packets, based on a large group of general and specific methods of solving Maxwell equations. The obtained quantitative and qualitative dependences for PCF Bragg fiber are similar to the other ones, for example [3], [7], [9]. This analytical method of calculation is a lot faster than the numerical ones, because of its simplicity.

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A NEW APPROACH TO THE CLASSIFICATION OF TECHNICAL CONDITION OF AIRCRAFT GAS TURBINE ENGINES IN THE COURSE OF THEIR LIFE CYCLE

НОВЫЙ ПОДХОД К КЛАССИФИКАЦИИ ТЕХНИЧЕСКИХ СОСТОЯНИЙ АВИАЦИОННЫХ ГАЗОТУРБИННЫХ ДВИГАТЕЛЕЙ В ПРОЦЕССЕ ИХ ЖИЗНЕННОГО ЦИКЛА

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Abstract: In this article is proposed a new approach to the classification of the technical state of aircraft gas turbine engines in the course of their life cycle. Given classification takes into account the occurrence of new kinds of technical conditions of the engine, which arises during the operation of aircraft equipment upon technical state. For faulty operating condition and for efficient operating condition is introduced the concept of critical and non-critical state. The article shows how is changing in the process of operation functionality of the engine, provided in the form of a curve with a characteristic areas and breakpoint for operation of the engine. This introduced breakpoint for operation of engine corresponds to its state before the failure state. There were introduced, on the basis of changes in the degree of functionality of the engine, certain technical conditions into which aircraft engines can enter and stay. The introduction of technical condition of the engine are described mathematically on theoretic-plural level. The article presents diagram of possible transitions from one engine technical state to another affected by both the operational and external control factors.

KEYWORDS: TECHNICAL STATE, GAS TURBINE ENGINE, FUNCTIONALY LEVEL, CONDITION MONITORING

1. Introduction

Aircraft engine consists of many systems, components, assemblies and parts, which in operation are exposed to a variety of factors and affect the technical condition of the engine. These factors are divided into two groups – the design-manufacturing and environmental ones. The first group of factors includes the selection of design schemes, materials, technologies, organization of production control, etc. The second group influences the technical condition of engine in operation. Subjective factors are associated with external actions from maintenance personnel; they can either enhance or decrease reliability. Objective factors reflect the operational conditions of the object, i.e., the impact from operating loads, the environment, etc. The environmental effect appears to change the object parameter values and characteristics in time, i.e., it manifests itself in deviation of parameters from their nominal values due to wear, ageing, maladjustments, etc. Due to diversity of environmental effects and their random character, the actual technical state of engine may be different within the same run time or length of operation. In general, the states that an engine may assume in operation as a technical object are certain transitions from one state to another as shown in [1]. As a rule, the initial state of the object is normal, i.e. it conforms to all the requirements of technical and design documentation. Any inconformity with these requirements transfers the object into a faulty state. As a result of damage or damages, the object (engine) may pass over from non-faulty state either to faulty operable state or faulty inoperable state, or, to the limiting state.

The faulty operable state is a state wherein the performance of all the preset functions is ensured (in full or in part) without going below the allowable safety and reliability level.

The faulty inoperable or just inoperable state is characterized by impairment of operability – a failure, i.e., the object's inability of performing the preset functions.

Both operable and inoperable objects may fall into the limiting state. A normal and operable object can pass over to the limiting state due to depletion of the specified life, obsolescence, or economic inexpediency of its further operation. Objects can be turned back to operation from the limiting state due to their recovery by repair contractors; at the same time, a profound upgrading or development may be performed. Inoperable objects fall into the limiting state if their recovery by and at the cost of a repair contractor is impossible, i.e., they need a repair, which will probably imply some engineering changes and developments. If the object recovery is impossible, it should be discarded or used as

something else; as for example, decommissioned aircraft engines are used in the national economy as power and gas installations.

2. Changing technical state of engine in operation

2.1. Change of engine functionality in operation

Modern strategies of operation of aircraft, such as the (Reliability Centered Maintenance) and CBM (Condition Based Maintenance) [2-5] are focused on the fact that the operation is provided up to the pre-failure conditions. Thus, monitoring and diagnostic systems must provide a prediction of pre-failure condition status of the engine, i.e., it should provide timely stopping of its operation.

Let us consider the problem where the possible technical states of engine as a whole and those of its systems, components, and assemblies will be specified more precisely. If we consider the engine state in terms of a change of its functionality within the “operable” time slot, i.e., before the failure took place, we can pinpoint some points and sections characterizing the engine functionality level in operation (Fig.2.1). The term “engine functionality” should be construed as the performance level of engine components and assemblies which ensure the engine application for the purpose specified under different flight modes and conditions.

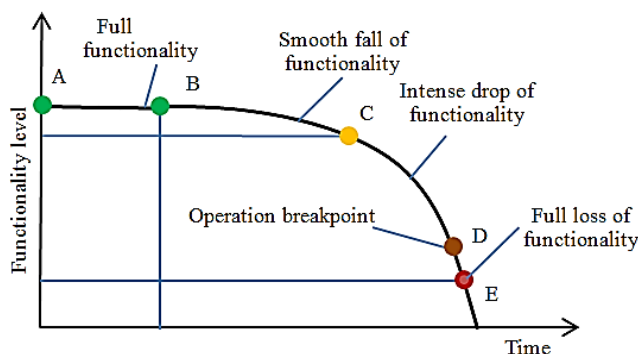


Fig.2.1. Change of engine functionality in operation

Within section AB, the object possesses full functionality, i.e. it is normal. At point B, functionality begins to fall; however, this fall is not critical one and the functionality still complies with standards,

which means that the engine is in operable state despite some faults not having a great impact on its functionality have taken place. With the accumulation of damage, the engine functionality begins to deteriorate more intensively until full loss of functionality, i.e. a failure, is reached at point E. Section CE in essence corresponds to pre-failure state of engine; therefore, the engine should be taken out of operation at this section with a view of doing recovery works. Point D at section CE will be the stop time or the time of the object removal from service; obviously, this point will be determined based on prognosis and with a certain probability.

2.2. Set-theoretic presentation of GTE technical state

Each functionality level of engine corresponds to a definite technical state of its components and systems, which can be described at set-theoretic level and presented in the form of Euler-Venn diagram (Fig. 2.2).

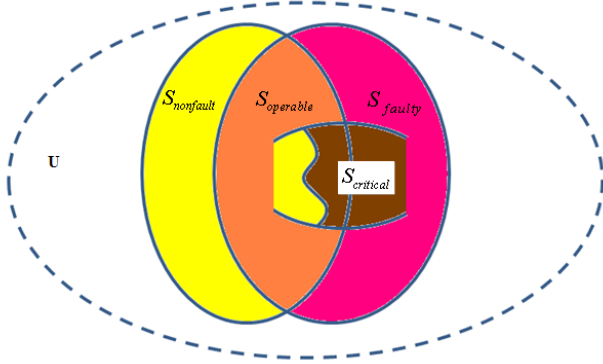


Fig.2.2. Graphical representation of the possible types of engines technical condition during operation

Set U of possible technical states of an engine (object) includes a set of non-faulty states $S_{nonfault}$ and faulty states S_{faulty} ; at the same time, the non-faulty state is always operable – $S_{operable}$. The intersection of the set of non-faulty states and the set of faulty states generates a set of operable non-faulty states $S_{operable}$. At the same time, an operable faulty state, in terms of its influence upon the engine reliability, may be uncritical $S_{uncritical}$ and critical (pre-failure) $S_{critical}$. Transition from critical to inoperable state (failure) is possible; however, if the object operability (non-faulty condition) cannot be recovered by virtue of operating company or this is impossible due to the complete object destruction – the object passes over to limiting state $S_{limiting_state}$. An engine may pass over to limiting state from operable/non-faulty state due to technical or economic inexpediency as well. Then, we can formulate it at set-theoretic level as follows:

- (1) $U \supset S_{reference_state} \stackrel{def}{=} S_{nonfault} \cup S_{faulty}$,
- (2) $S_{nonfault} \cap S_{faulty} \stackrel{def}{=} S_{operable} \neq \emptyset$,
- (3) $S_{nonfault} \not\subseteq S_{faulty}$;
- (4) $S_{nonfault} \stackrel{def}{=} S_{perfect} \cup S_{operable}$, $S_{perfect} \cap S_{operable} = \emptyset$
- (5) $S_{operable} \stackrel{def}{=} S_{uncritical} \cup S_{critical}$, $S_{uncritical} \cap S_{critical} = \emptyset$
- (6) $S_{critical} \stackrel{def}{=} (CA[S'_{critical}] \vee P[S'_{critical}]) \cup P[S''_{critical}]$,
 $\stackrel{def}{=} S_{perfect} \subseteq S_{critical}$
- (7) $S_{perfect} \cap P[S''_{critical}] = \emptyset$, $\forall S'_{critical} \subseteq S_{critical}$,
- (8) $S''_{critical} \subseteq S_{critical}$;

- (9) $S_{limiting_state} \stackrel{def}{=} P[S''_{critical}] \cup S_{other_capacity/spares} \cup S'_{retirement}$,
 $\forall S'_{retirement} \subseteq S_{retirement}$;
- (10) $S_{limiting_state} \stackrel{def}{=} P[S''_{critical}] \cup S_{other_capacity/spares} \cup S'_{retirement}$,
 $\forall S'_{retirement} \subseteq S_{retirement}$;
- (11) $S_{uncritical} \stackrel{def}{=} (S_{nonfault} \square S_{faulty}) / S_{critical}$

We introduced here, that set $CA[\cdot]$ is generated by operator action CA (control actions) on subset $[\cdot]$ of set $S_{critical}$, while set $P[\cdot]$ is generated by operator action P (preparatory works) upon subset $[\cdot]$ of set $S_{critical}$.

The engine falling into the technical states shown above can be described as a random (stochastic) process $X(t)$; one of the models of this process [58] is formulated as

$$(12) \quad X(t) = A(t) + X_e(t),$$

where $A(t)$ is a determinate, continuously differentiable function, while $X_e(t)$ is a stationary ergodic normal process with zero mean. To predict the transitions of process $X(t)$ from one state to another, a certain supporting process

$$(13) \quad Y(t) = A(t) + Y_e(t)$$

is used, where $Y_e(t)$ – predictor for $X_e(t)$, calculated at the moment $(t - m)$; at that, $m > 0$ will be a certain selected variable. If the value $Y(t)$ calculated at the moment $(t - m)$ exceeds a certain critical value $\hat{u}$, then a warning message about a possibility of process $X(t)$ overrunning level $u(\hat{u} < u)$ at the moment t .

3. Classification of GTD technical states during the process of operation

Traditionally, are distinguished serviceable and fault states, wherein fault conditions are distinguish operable and inoperable states [6]. In diagnostic practice, in general, quite often distinguish only two states – operable and inoperable. This approach is quite simplistic and mismatches principles of modern strategies of exploitation of aircraft.

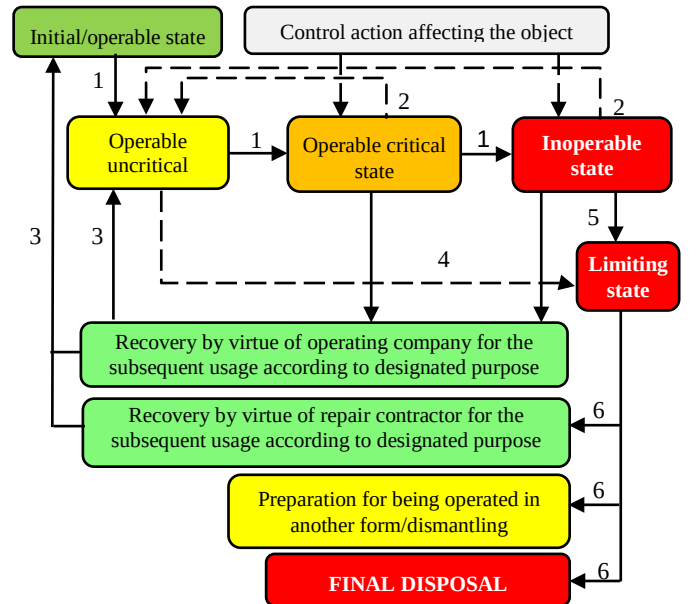


Fig.3.1. Cognitive graphical scheme of service engine transitions from one state to another: 1 – damage accumulation; 2 – performance restoration under control action; 3 – operational performance restoration; 4 – depletion of specified life, economical or technical inexpediency; 5 – full loss of functionality; 6 – possible transitions from limiting state

Thus, observing the process of a change of technical state of engine, we can trace the actual current state of the engine and, respectively, schedule maintenance and repair operations. The process of engine transitions from one state to another in operation may be presented in the form of a graphical scheme (Fig.3.1).

The scheme presents the dynamics of possible states of GTE throughout its lifecycle. On damage accumulation, the engine passes over sequentially from non-faulty to operable uncritical state, then to critical state and, finally, loss of operability, i.e., failure is reached. The engine can be recovered from critical and inoperable states to operable state if a control action is applied – like for instance, change of the engine operation mode or passing over to emergency or backup control, leaving the boundaries of an adverse weather zone etc. In this case, we may speak of a temporary recovery of engine operability in an emergency.

If the damages received by engine are essential, which leads to engine decommissioning for an indefinite time – such a state is considered to be limiting. An engine can be transferred to the limiting state on depletion of its specified service time as well, or, its further operation as intended is technically or economically inexpedient. On getting into limiting state, engine can be restored to non-faulty state; it can also be redesigned for a different function, or commissioned. The scheme gives a clear idea of the possible states of engine and the understanding of what actions should be taken in operation.

3. Conclusion

Modern aircraft operation strategy aimed at reducing operating costs and maintaining reliability at a safe level. The modern means of monitoring and diagnostics of technical state allows to determine and predict the actual technical condition of the engine. Therefore, the proposed classification of the technical states of the engine makes it possible to display, more accurately. The actual technical state in which may be the engine during operation.

The developed scheme of transitions of the engine from one technical state to another clearly shows how changes occurs in technical condition throughout the life cycle of the engine.

This article also presents a mathematical description of the theoretic-plural level of possible technical states and their transitions from one state to another

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APPLICATION OF INTERACTIVE ONLINE TOOLS OiRA FOR RISK ASSESSMENT OF WASTEWATER TREATMENT

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Abstract: Economic activity "collection, disposal and treatment of waste water" is especially risky in terms of working conditions. A significant proportion of workers in this activity are regularly exposed to humidity and low temperatures. Particularly significant and causing serious damage to the health of employees impact of materials that can cause infectious diseases. Additional physical and psychological stress has and the fact that employees must comply with stringent quality standards. In order to facilitate the risk assessment process, the European Agency for Safety and Health at Work – Bilbao (EU-OSHA) has developed a comprehensive user-friendly free web application, OiRA (an interactive risk assessment online tool), which helps micro and small enterprises to perform an overall step-by-step risk assessment – from identifying and assessing risks at work, making and implementing decisions on preventive measures, to continuous monitoring and reporting.

Keywords: COLLECTION, DISPOSAL, TREATMENT, WASTE WATER, RISK ASSESSMENT, OiRA

1. Introduction

The business sector "Waste water collection, disposal and treatment" is one of the most risky in terms of working conditions. A great number of workers performing this job are regularly exposed to humidity and low temperatures. The impact of materials which may cause infections plays a crucial role and can severely affect their health. Those workers have to meet very strict quality standards, which brings additional physical and psychological burdens.

A number of factors of the working environment have a negative effect on the workers in this sector. Their job is often monotonous. They spend much of their working hours standing or walking. These risks come from the specific nature of the job and their influence can hardly be eliminated. Therefore, the employers in the area of waste water collection, disposal and treatment should organize the work of their employees in such a way that the possible risks for the health of the latter and the occurring consequences should be reduced to a maximum. A great number of the employees in the above mentioned area work 50 hours a week. In addition, many employees work at night and on Sundays. This is a result of the 24-hour manufacturing cycle in this sector.

The prevailing health problems among those employees are fatigue, muscle pains, headaches, vision problems. Many of them report about breathing problems. The employees spend some working hours underground in a wet and humid environment.

One of the risks is linked to the type of the waste water treatment plant, as well as to the various chemicals used in the respective processes. Taking into account the above mentioned, health hazards can be classified into three categories: physical, chemical and microbiological.

The specific nature and variety of the manufacturing processes related to the waste water collection, disposal and treatment result in a relatively high risk of occupational accidents and diseases. Actually the data obtained from the National Social Security Institute show that the number of the occupational accidents in this business sector is low. However, due to the small number of employees in the field of waste water collection, disposal and treatment the coefficient of frequency of occupational accidents is higher than the country average.

Risk assessment is an important first step in the prevention of occupational accidents and diseases. OiRA, an online interactive risk assessment tool, facilitates this process. OiRA provides step-by-step solutions to the risk assessment process – it starts by defining the risks at work, then it gets users acquainted with the process of implementation of preventive measures, and it ends with monitoring and risks reporting. [1]

2. Explanatory

In order to facilitate the risk assessment process, the European Agency for Safety and Health at Work – Bilbao (EU-OSHA) has developed a comprehensive user-friendly free web application, OiRA (an interactive risk assessment online tool), which helps micro and small enterprises to perform an overall step-by-step risk assessment – from identifying and assessing risks at work, making and implementing decisions on preventive measures, to continuous monitoring and reporting. OiRa is based on the successful Dutch RI&E tool. [2] All tools are available free at <http://www.oiraproject.eu/available-tools/#mainContent#title>.

Each risk assessment performed by OiRA follows the steps below:

1. Preparation;
2. Definition;
3. Assessment;
4. Action Plan;
5. Report.

1. Preparation

Depending on the tool structure (Fig. 1), the following is required during this step:

- Choose or skip a situation/situations depending on whether they are important for your business.
- List identical structural units, branches, shops, etc. For each of these identical structures identical risk assessments will be prepared within the next steps.

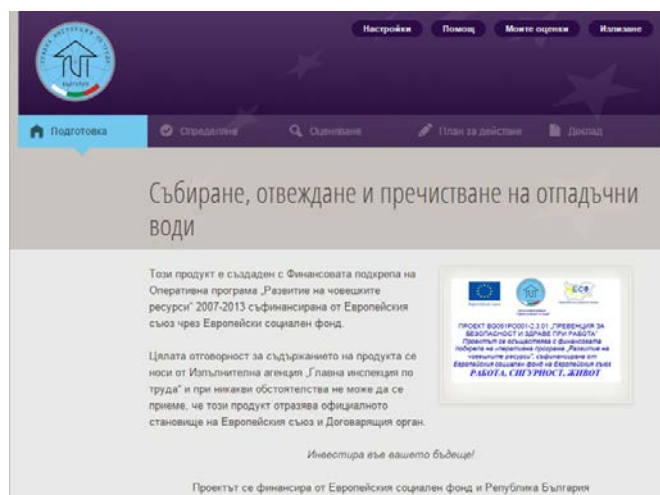


Fig. 1. Preparing for risk assessment OiRA

2. Definition

Within this step the specific dangers and problems in the enterprise are defined. (Fig. 2)

The type of the single groups of dangers that will be defined is structured in modules and sub-modules. The module content is in compliance with the requirements of art. 3 of Ordinance 5 on the Procedure, Manner and Frequency of Carrying Out Risk Assessment. [3]

The importance and topicality of the modules and their scope are confirmed by the results presented in the Profile of Safety at Work “Waste water collection, disposal and treatment”.

Each module contains a database of statements describing the risks for the employees and the following principles are observed: /if the statement is true, the risk is permissible and vice versa/, and when the regulatory requirement is not met, the risk is non-permissible.

Some of the risks are defined by default and can not be changed, for example the risk of falls from an elevation is always high and can not be changed.

For each statement explanations about the risk and its causes are provided (danger, regulatory requirement and other risk-related information).

Basic/principle solutions applicable to waste water collection, disposal and treatment are given.

The statements are formulated in such a way that the possible answers are “YES” or “NO”.

Fig. 2. Risk assessment

3. Assessment

Within this step the risks caused by the dangers/problems determined in the Definition step are assessed, as well as the level of these risks (Fig. 3). Depending on the envisaged assessment method, the following has to be done for each risk:

- To make a decision on its priority: high, medium and low.
- To determine the variables (exposure, weight of the harm and probability) so that the system can automatically calculate the risk priority according to your settings.

This result will be shown in the Action Plan step.

Some risks are very important and have very serious consequences therefore it is not necessary to assess them. They will be considered in the Action Plan step.

Fig. 3. Assessing the identified risks

4. Action Plan

Within this step a decision about the measures that can be taken to eliminate or minimize the risks defined is made. (Fig. 4)

Additional measures can be entered and/or measures proposed by the system can be selected. In addition, the proposed measures can be changed.

The following should be completed for each measure:

- The overall approach (to eliminate or minimize the risk).
- The specific action/s required for the application of the respective approach.
- The required level of expert experience and/or requirements.
- The person responsible: the person responsible for the implementation
- The budget: the costs to be incurred.
- The start and end date.

Fig. 4. Preparation of an action plan

5. Report

By means of the Report you can check the implementation of the Action Plan and its current status at any time. It is useful because it monitors and reports to the Safety Councils how the planned measures are implemented and if necessary to correct the initially planned actions and the adopted deadlines. (Fig. 5)

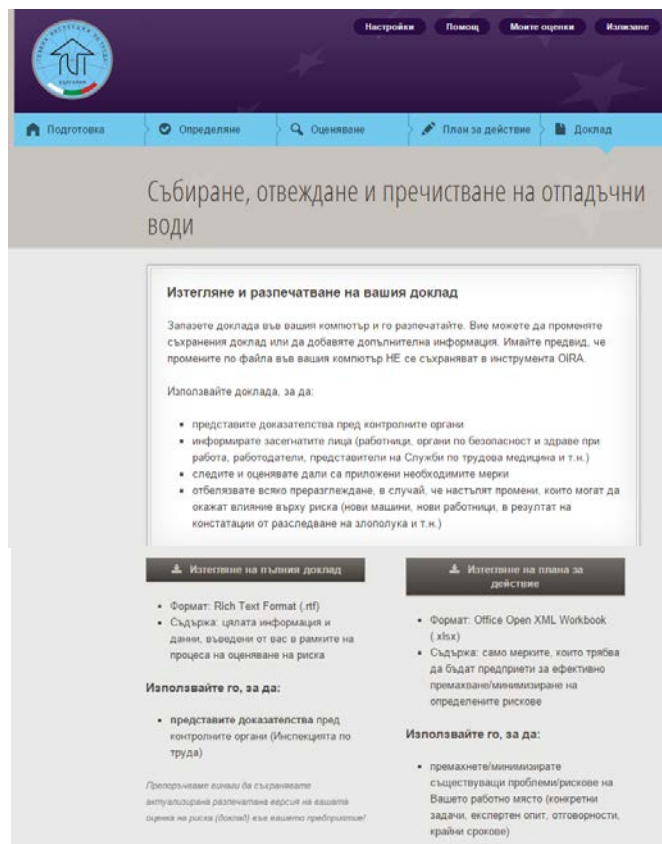


Fig. 3. Finalize the report and plan and opportunities for its treatment

The Report is a very important and useful element of the OiRA tool since the conditions under which the work is done constantly change and the risk assessment should be continuously updated and adapted to the new working conditions.

The Report can justify the necessity for updating the Health and Safety Plan in relation to new emerging risks in the course of work.

3. Conclusion

The benefits of the OiRA risk assessment tool are as follows:

- The process of risk assessment or assessment review can be stopped and restarted at any time.
- The online assessment is securely stored and protected by a password. It can be accessed at any time by the person who created it in order to review or update it by editing the records.
- It can be used by less experienced people who are not experts in the area of Safety and Health at Work. It unifies the approach of risk assessment by comprising minimal requirements to provide health and safety at work.
- It is user-friendly and allows us to increase the information integrated in it in order to help the assessors. Therefore, it is also useful for experts in the field of health and safety at work.
- The Action Plan and the Report can be printed at any time so as to document the assessment results.
- One user can create an unlimited number of assessments for different enterprises and subjects.

- An already created assessment for a given subject after its change can be adapted to another analogous one. In this way the time for repeating already assessed situations is saved.

The contents of interactive online tools for risk assessment OiRA part of the economic activities is created by the authors within the project BG051PO001-2.3.01 "Prevention Safety and Health at Work" implemented with the financial support of OP "Human Resources Development" co-financed by the ESF EU and implemented by EA "GLI".

Additional information is available at:
<http://projects.gli.government.bg/>

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CURRENT STATE AND DEVELOPMENT PROSPECTS OF METHODS TO INCREASE THE STRENGTH AND DURABILITY OF THE CYLINDRICAL THIN-WALLED ELEMENTS

СОВРЕМЕННОЕ СОСТОЯНИЕ И ПЕРСПЕКТИВЫ РАЗВИТИЯ МЕТОДОВ ПОВЫШЕНИЯ ПРОЧНОСТИ И ДОЛГОВЕЧНОСТИ ТОНКОСТЕННЫХ ЦИЛИНДРИЧЕСКИХ ДЕТАЛЕЙ

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Abstract: The main issues are considered in this topic is the impact of pneumovortex effect on the free ball located inside the cylindrical thin-walled elements. Researches were carried out with various diameters of deforming balls and lengths of cylindrical parts. Obtained results show high precision of roughness inside walls of cylindrical tubes.

KEYWORDS: FINISHING-STRENGTHENING, PNEUMOVORTICAL PROCESSING, DISTORTING BALLS, ROUGHNESS

1 Introduction

Nowadays the ball rolling is widely used for finishing-strengthening treatment of non-rigid elements parts, which provides to receive high specific pressure to the wall parts with less effort. However, the main condition of reliable operation of such rolling-off is a high precision in production. Increased requirements to accuracy of hole-rolling processing, even in small oscillations of tension, lead to a drastic change of efforts and the angle pressing in of distorting elements, which has an adverse effect on quality of thin-walled elements. Furthermore, the use of roller burnishing tool does not supply high-performance process.

On the other hand there are examples of use of known methods, applied to the cylindrical thin-walled elements (cold cathode substrate) made of viscose steels and alloys in some factories of engineering and electronics industries.

2 Solution of the problem

However, technological losses at processing of the thin-walled cylindrical parts using the method of rolling by distorting ball are more than 10 % [1]. These losses arise at “tough” contact of distorting element with work detail owing to charging surface, change of geometry of the detail and non-uniformity of distribution of processing efforts. Besides small rigidity and vibration resistance of the system results in occurrence of defects as sections with high sizes of the surface roughness having random nature of distribution.

On the basis of our theoretical and experimental research has developed a number of device constructions for pneumovortical processing of cylindrical elements.

At pneumovortical process distorting balls, committing complex motion regarding work surface interact with microasperities of the initial surface in various directions [2].

Rolling microasperities occurs on different sides, whereby the deformation resistance decreases, and the deforming action of the balls increase during this motion. The resulting component flow pushes the ball constantly with a certain force to the surface at an angle of ascent respect to the axis normal of the cylindrical element (Figure 1).

However, factors such as turbulence of the vortex flow, surface roughness, loss of energy flow along the length of the workpiece, the contact friction and weight of the ball prevent the latter to move up on the surface incrementally, which provides required roughness of the finished product. Hence, above mentioned factors do not allow the ball to contact with all microasperities of the initial surface.

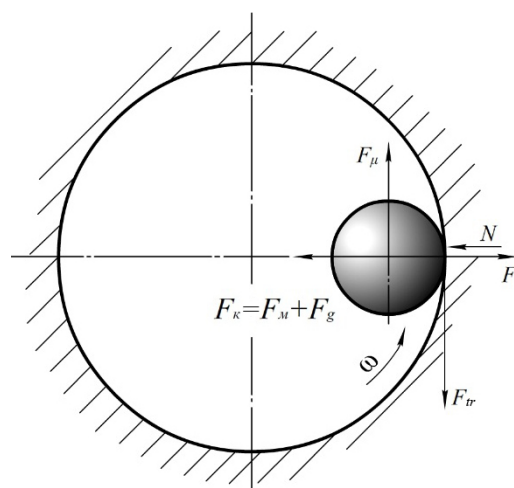


Figure 1 Forces at the contact point of the ball and cylindrical tube

The deforming balls contact with the entire work surface can be achieved by increasing their number. It is necessary to find a combination between control parameters (P_v , d_{ub} , N_{ub}) that would supply the required quality of the surface along the whole length of workpiece.

3 Experiment, Results and Analysis

As the deformation elements were chosen polished steel balls of material IX-15 with diameter range $d_{ub} = 1,6 \div 3,5$ mm; in an amount of $n = 10 \div 300$. The input pressure was selected within $P_v = 0,2 \div 0,35$ MPa. Output parameters of workpiece and output of devices of pneumovortical processing to a large extent is defined of following parameters: the initial surface roughness, diameter and length of workpiece and control parameters.

The results of experimental researches are plotted in fig. 2. It can be seen that the more rough the initial surface before lining-reinforcing processing, the easier to achieve a sharp improvement of the surface roughness in the beginning.

For example, at the initial roughness $R_{init} = 5,0 \div 6,0$ mcm, (the elements' material is Д16Т) for initial time of processing $t = 1,5$ minutes R_z decreased on $\Delta R = 4,6$ mcm at the initial $R_{init} = 1,25$ mcm, for the time of processing roughness decreased $\Delta R = 1,0$ mcm.

Besides at any initial surface of preparation the curve of change R_a of processed detail at increase of the time of processing asymptotical seeks some size.

At the initial roughness $R_{init} = 5,0 \div 6,0$ mcm value asymptote averages 0,18 mcm, and at the initial roughness $R_{init} = 1,25$ mcm value asymptote - 0,12 mcm.

Such nature of processing the balls contact with work surface on the tops of micro roughness, reference area of which is small. Thereof on contact surface significant specific pressure causing plastic deformation of micro roughness develop. However hereinafter contact takes place to big reference area. Besides to quality of processing they begin to influence arising wear hardening of the surface and occurrence of defect layer. All of these results in reduction of power impact increase of strength of the surface and, as investigation, slow change of roughness in time.

Seeking to increase impact of balls to surface at the expense of increases of entrance pressure higher that recommended results in destruction of surface layer, occurrence of scores and hollows.

In such a manner, such initial roughness of preparation is possible that even with infinite the time of processes we will not receive required quality of the surface (surface roughness $R_a=0,1\div 0,08$ mcm).

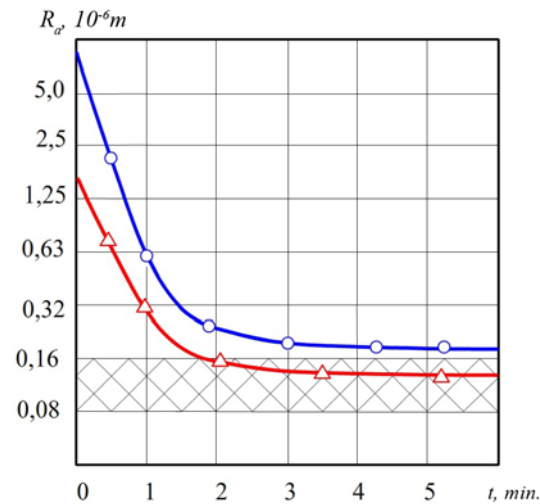


Figure 2 Influence of duration of processing to roughness at various R_{init} :
 $\bigcirc$ - $R_{init}=5,0$ mcm; $\triangle$ - $R_{init}=1,25$ mcm

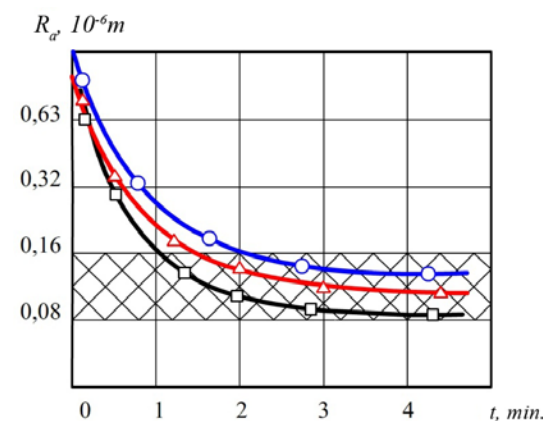


Figure 3 Influence of duration of processing to roughness at different diameters and lengths of workpiece
 $\bigcirc$ - $D_n=40$ mm, $L=200$ mm; $\square$ - $D_n=40$ mm, $L=160$ mm;
 $\triangle$ - $D_n=40$ mm, $L=160$ mm

For the above mentioned parameters of the device and the modes of processing at required roughness of vendor part $R_a=0,16\div 0,08$ mcm receipt of required quality is possible only in case semi-finished items surface roughness will be less size $R_{ini}<0,3$ MPa mcm.

Based on above-stated, it is recommended the initial detail roughness to choose within the range of $R_{ini}=0,63\div 2,5$ mcm. At the same time processing will long for $2\div 3$ minutes.

In fig. 2 the results of research in influence of processing duration to surface roughness are presented at different diameters and lengths of workpiece. For example, increase of length of the cylindrical elements from $L=160$ mm to $L=200$ mm at diameter of the element $D_n=40$ mm results in increase of the time of processing

with $t=2,5$ to $t=3$ minutes, and for element with $D_n=30$ mm and length $L=120$ mm processing time accounts for already $t=2,0$ minutes. It is due to that with increase of length and diameter of workpiece the way passed by the ball during processing is increased, and therefore, duration of processing grows.

Excessive increase of requirements to quality of the semi-finished items surface though results in processing time reduction, but much will increase expenditures to previous operations.

Other advantage of thin-walled cylindrical elements is opportunity of formation of optimum microrelief (uniformity of surface layer) and significant hardening of surface layer of metal without deformation of preparation on her all section.

On fig. 4 they are presented in profilograms, obtained from the surfaces of work piece (elements' material is Д16Т) recorded on profilograph - profilometer 201, at identical vertical and horizontal increases. Profilogram (fig. 4, a) corresponds condition after passage on the machine tool of the model 1И611П (roughness on parameter $R_a=1,25\div 0,63$ mcm), and profilograms (fig. 4 b, c) condition after lining-reinforcing processing at duration of processing, respectively $t=2$ and $t=3$ minutes is corresponded (roughness on parameter $R_a=0,16\div 0,08$ mcm)

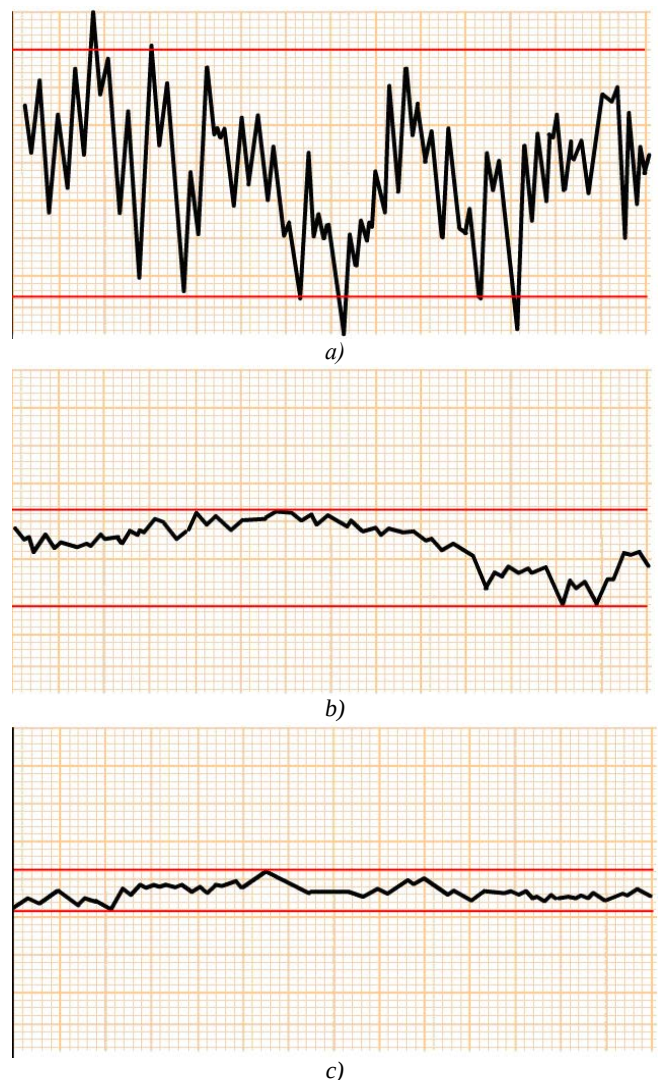


Figure 4 Nature of the surface roughness of work detail after:
a) passages on the machine tool of the model 1И611П;
b) lining-reinforcing processing of pneumovortical action at duration of processing respectively $t=2$ m and $t=3$ m.

As exemplified by received profilograms the microrelief of processed detail surface by method of lining-reinforcing processing of pneumovortical has an insignificant amount of shallow grooves, projections smoothed form have, and surface roughness R_a does not exceed $0,16\div 0,08$ mcm. Such surface supplies an almost ideal

distribution of the current in the class to the area of the cathode and satisfies to all requirements imposed on work detail after operation roller.

4 Conclusions

In such way, the strengthening effect produced by finishing and hardening treatment is not only the value of power impact of the ball on the surface, but also due to load annex ratio to surface and complex relative movement of distorting ball regarding the workpiece.

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METHODOLOGY FOR OPTIMIZING THE INFLUENCE OF SURFACE ROUGHNESS ON THE FUNCTIONAL PROPERTIES OF DETAILS IN MECHANICAL ENGINEERING

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Abstract: The article deals with a fundamentally new methodology for optimization, assessment, and control of the roughness of surfaces that can be applied in all production facilities. What is meant by optimization is the choice of the most appropriate roughness from among all the practically possible values that can be achieved in certain production conditions. The given methodology is used as a basis for the assessment of the influence of surface roughness on the strength of a joint formed through the process of hot pressing.

Keywords: SURFACE ROUGHNESS, NON-PARAMETRIC METHOD, STENGHT OF PRESS JOINTS

1. Introduction

Improving the quality of output production is the most important task of industry [1]. This task is especially relevant in machine-building and mechanical engineering. It is general knowledge that the correct functioning of every item is determined by its accurate size, the shapes, and the proper positioning of the contact surfaces of its parts, as well as the state of their surface. The least researched areas are problems related to the optimization of the micro geometry of surfaces and providing reliable control.

So far, it has been established that surface roughness has a direct bearing on about 20 functional properties of surfaces (adhesion, corrosion resistance, strength of press joints, etc.). Modern-day machinery requires coping with a number of challenges related to increasing the strength and improving the efficiency of machine parts and constructions, including the fixed joints [2]. This necessitates a thorough analysis to study the effect of a number of factors on the strength of press joints – geometric factors, the macro and micro relief of the contact surfaces of machine parts, the physical and chemical properties of the materials that the parts are made of under the specific conditions of forming the joints.

It is a known fact that the load-bearing capability of press joints is determined by their ability to withstand certain loads (torque or axis force). The quality of the joints is determined to a large extent by the geometry of the contact surfaces of the machine parts. Many of the published studies [3,4] suggest increasing the strength of press joints through applying a regular or partially regular micro relief on one of the machine parts. It is suggested that the process be performed through surface plastic deformation or the creation of micro relief on two levels by means of making curvilinear grooves in the stick. The most significant drawback of the above mentioned methods are the complexity of the relief-making tool, the difficulties arising from providing accurate orientation of the grooves and the projections of the micro relief, and the relatively low productivity of the process.

The article elaborates on a fundamentally new methodology for optimization, assessment, and control of the surface roughness, applicable in all types of production situations [5-8]. What is meant by optimization is the choice of the most appropriate roughness from among all the practically possible values that can be achieved in certain production conditions. The given methodology is used as a basis for the assessment of the influence of surface roughness on the strength of a joint formed through the process of hot pressing.

2. Definition of the task

A joint [7] produced through the process of hot pressing is taken as an example (fig.1).

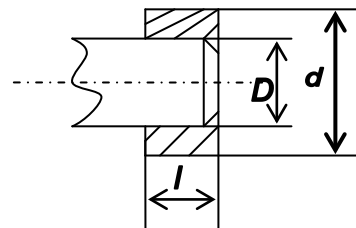


Fig. 1 A hot-pressed joint with a nominal diameter of contact area $D = 20$ mm, external diameter of the threaded collar $d = 30$ mm, length of contact area $l = 20$ mm. Under exploitation the joint is loaded with axis force $F = 6,65 \cdot 10^3$ N.

In order to study the effect of surface roughness on the strength of the press joints, we have prepared 9 samples, in three groups of three pieces depending on the obtained surface roughness. The samples in the first group were produced through turning, with the resulting surface roughness of the shaft and threaded collar are respectively: $R_{z \text{ threaded collar}} = 15,04 \mu\text{m}$ and $R_{z \text{ shaft}} = 17,64 \mu\text{m}$. In the second group – through grinding: $R_{z \text{ shaft}} = 1,269 \mu\text{m}$ and $R_{z \text{ threaded collar}} = 10,05 \mu\text{m}$, and in the third group – through polishing: $R_{z \text{ shaft}} = 2,1 \mu\text{m}$ and $R_{z \text{ threaded collar}} = 2,65 \mu\text{m}$.

In order to test the strength of the produced joints, they were subjected to un-pressing, through fixation of the load. The result of the testing is this: the samples in the third group show un-pressing load of $F = 26 \cdot 10^3$ N, which is 20 % more than the un-pressing load of the samples in the second group with the same force, and 50% more than the samples in the first group under the same conditions.

3. Theoretical analysis of the chosen method

The results show the considerable effect of the surface roughness on the force applied to un-press the joints. This proves the expediency of optimizing this effect.

But the task of optimizing the roughness of surfaces cannot be plausibly achieved with the use of the standard parameters for roughness because their alteration does not characterize the factual alteration of the micro relief of the surfaces [5-8]. In order to achieve the preferred parameter for roughness that has been experimentally selected and designed in the draft, either different technologies or different tools can be used to implement a change in the structure of the micro relief and consequently in the properties of the surfaces. Setting a specific parameter for roughness in the technical documentation, we would be able, in aiming to achieve it, to process the surface in a way that will lead to one of the many possible micro reliefs which will provide different functional properties. Most methods of processing surfaces yield a random pattern of roughness. This is why, in modeling the

roughness of surfaces, the theory of random functions can be used, which in effect implies that the pattern of roughness of a given surface can be viewed as the realization of a random value. And we all know from mathematics that the full parametric definition of a random value requires 3 to 25 parameters – and this is exactly as many parameters of roughness as need to be specified in the construction draft in order to provide an exact definition of the required roughness. Theoretically this is possible, but in practice this is hardly feasible.

A possible solution for this situation is suggested in one fundamentally new approach for assessment and control of the roughness of surfaces – a method which uses non-parametric criteria such as the diagrams of different functions [1,5,6,7,8]. Taking into account the random element in forming the micro relief of surfaces, and based on the theory of random functions, it has been established that the most comprehensive information about the pattern of roughness as a random value is contained in the functions of distribution and the density of distribution of its ordinates, as well as in the functions of distribution and the density of distribution of the tangents from the angles of inclination of the pattern. This naturally leads to the conclusion that it is expedient to use these functions as criteria for the assessment and control of the roughness of surfaces.

In line with the proposed methodology, below are the diagrams of the non-parametric criteria “Density of distribution of the tangents from the angles of inclination of the pattern” that were made with the samples under analysis.

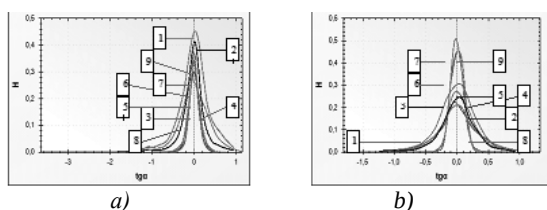


Fig. 2 Diagrams of the non-parametric criteria “Density of distribution of the tangents from the angles of inclination of the pattern”: a) for the threaded collars, b) for the shafts.

The numbers in the diagram show the numbers of the studied samples (1 through 3 – first group, 2 through 5 – second group, 6 through 9 – third group).

4. Analysis of the results

The experiment that was conducted shows that the roughness of surfaces affects the strength of press joints, which proves the expediency of optimizing this effect. The process of optimization is done through trying to find the optimal level of the functional property (optimization parameter) by varying the technological modes of processing (optimization factors) [9]. The force of un-pressing the joints (F) is considered a parameter for optimization, with the optimal level being the highest possible value. The factors of optimization are the modes of processing in polishing the machine parts “shaft” and “threaded collar”: $S_{threaded\ collar}$ – use of one rotation in polishing the threaded collar, $V_{threaded\ collar}$ – velocity of cutting in polishing the threaded collar, S_{shaft} – use of one rotation in polishing the shaft, V_{shaft} – velocity of cutting in polishing the shaft. After conducting a statistical regression analysis, on the basis of the theory of planning the experiment, the following data was arrived at:

- a mathematical model relating the optimization parameter with the technological modes of processing and making it possible to forecast the level of force required for un-pressing with variations of the above-mentioned factors

$$F = 17,25 - 3,5S_{threaded\ collar} + 2,5V_{threaded\ collar} - 1,25S_{shaft} + V_{shaft} + 0,8S_{threaded\ collar}V_{threaded\ collar}S_{shaft}V_{shaft}$$

- technological modes of processing which produce an optimal surface roughness, guaranteeing the highest level of force required for un-pressing $S_{threaded\ collar} = 0,43\ m/min$, $V_{threaded\ collar} = 37,5\ m/s$, $S_{shaft} = 0,467\ m/min$, $V_{shaft} = 36\ m/s$

- optimal surface roughness of the following machine parts «Threaded collar» and «Shaft», which can be controlled through the use of non-parametric criteria presented in fig. 3 – these are the reference diagrams and the tolerances.

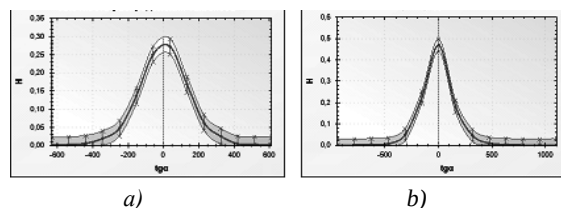


Fig. 3 Reference diagrams «Density of distribution of the tangents from the angles of inclination of the pattern» with an indication of the tolerance for: a) the threaded collars, b) the shafts

These curves, assumed as reference curves, are related to the sample surfaces that showed the best results in the course of the experiment. It is possible that there exist other surface roughness values which can require greater load for un-pressing and, therefore, greater strength of the press joints, but the present article’s aim is to define the best geometry that can be achieved under specific production conditions.

5. Conclusion

The use of standard parameters to assess and control the surface roughness of machine parts, appliances and machines has only one advantage – the simplicity of its practical use [6]. When we are looking for a complex criterion dependent on several factors, it is simply impossible to apply numerical criteria because they do not allow for the optimal characteristic (the most appropriate of all the possible ones) of the normed functional property of the surface to be accurately defined with a practicable degree of accuracy. The functions of density of distribution and the functions of distribution of ordinates and tangents of the angles of inclination of the pattern unequivocally define the roughness of surfaces and fully satisfy the legitimate requirement of a thorough and comprehensive definition.

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SURFACE ACTIVITY OF SOLUTIONS FOR ELIMINATING RADIOACTIVE CONTAMINATION

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Abstract: Surface activity of water solutions, surfactants, has been calculated on the base of concentration dependence of surface tension. Compounds for deactivation, based on synthetic detergents in different concentration scales have been offered.

Keywords: SURFACE TENSION, SURFACTANTS

1. Introduction

The deactivating solutions, applicable to eliminate radioactive contamination are mainly required to have enough wettability for the processed surfaces. Surface activity is quantitative and qualitative criterion of deactivation solutions wettability and it is also a temperature dependent quantity. It has been defined by Gibbs absorption isotherm.

$$(1) \quad \alpha = -\frac{C}{RT} \left(\frac{\partial \sigma}{\partial C} \right)_A,$$

where: α is surface adsorption concentration, mol/g; C – concentration of solution, mol/l; R – universal gas constant, J/mol.K, $R=8,3$ J/mol.K; A – surface of processed area, m²; $g = \left(\frac{\partial \sigma}{\partial C} \right)_A$ – surface/ capillary/ activity.

The quantity $\left(\frac{\partial \sigma}{\partial C} \right)$ can have different signs. For surfactants $\left(\frac{\partial \sigma}{\partial C} \right)_A$ it is minus sign, hence for surfactants $\alpha > 0$ the adsorption on the surface of the solution is positive.

Water solutions of surfactants are used for conducting deactivation. In the Bulgarian Army the composition DV-2 is in use, it contains alkylphenolpolyglycol ethers, sodium triphosphosphate and sodium sulphate.

The objective of this research is to be carried out comparative analysis on the wettability of two kinds of solutions: on the one hand - water solutions, containing DV-2, and on the other hand water solutions on synthetic detergents, which can be used for deactivation in different temperature and concentration interval.

2. Measurement Methodology and Research Object

Objects of the research are water solutions DV-2, water solutions of SHTAMEX, or powder-like synthetic detergents on the base of sodium salt of alkyl derivatives of benzene sulphaicid (containing 10-16 carbon atoms). The names – synthetic detergents SD „T” [4] and SD „B” [5] are introduced figuratively. Their components are given in Table1. Shtamex is a composition which is applicable in extinguishing fires by Fire Security and population protection.

Table 1: Synthetic detergents components.

Ingredients of SD „B”	Ingredients of SD „T”
- 5÷15% sodium salt of alkyl derivatives of benzene sulphaicid (containing C ₁₀₋₁₆)	- 5÷15% sodium salt of alkyl derivatives of benzene sulphaicid (containing C ₁₀₋₁₃);
- 10÷20% sodium carbonate	- 5÷15% sodium carbonate;
- 1÷ 5% C ₆ H ₅ O ₇ /CH ₂ COOH-C(OH)COOH-CH ₂ COOH	- <5% polyacrylic acid;
5 ÷ 15% sodium silicate	- 5÷15% sodium silicate.

The research has been conducted in a concentration range from 0,1% to 0,35%. To calculate the surface activity it is necessary to be aware of the correlation $\sigma = f(C)$, which can be received experimentally.

Defining surface tension is completed through the method of maximum pressure while blowing a bubble from the capillary. [1,2,3]. The correlation between surface activity and temperature is fixed indirectly using the data of surface tension dependence on temperature. Heating the samples of experimental solutions is realized indirectly with heated in thermostat water, used as heat carrier. [1, 2]

The amounts of studied objects’ surface activity are defined with graphic differentiation of $\sigma = f(C)$ correlation, applying computer platform [6]. Figure 2 is a chart of example correlation $\sigma = f(C)$, showing:

$$(2) \quad \operatorname{tg} \varphi = \frac{\partial \sigma}{\partial C} = g,$$

where: g – surface activity; $\partial \sigma$ – infinitely small change in surface tension, ∂C – infinitely small change in concentration.

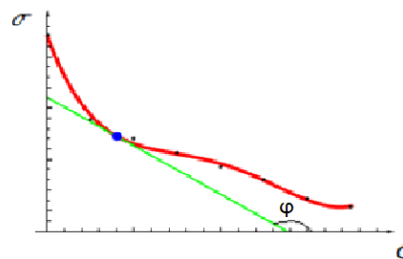


Fig. 1 Graphic chart $\sigma = f(c)$ for defining surface activity of solutions.

3. Results and discussion

Fig. 2 illustrates correlations $\sigma = f(c)$ for DV-2, SD „T”, SD „B” and „SHTAMEX” at temperature of 20°C. Statistically processed data of correlations $\sigma = f(c)$ [6] respectively for DV-2, SD „T”, SD „B” and „SHTAMEX” at (3), (4), (5) and (6) are given with regression equations:

$$(3) \quad \sigma = 0,073 - 0,072.C + 0,539.C^2 - 2,842.C^3 + 3,849.C^4$$

$$(4) \quad \sigma = 0,073 - 0,215.C + 1,061.C^2 - 3,389.C^3 + 4,153.C^4$$

$$(5) \quad \sigma = 0,072 - 0,449.C + 3,457.C^2 - 12,776.C^3 + 16,849.C^4$$

$$(6) \quad \sigma = 0,072 - 0,027.C - 0,010.C^2 - 0,001.C^3$$

where: σ – surface tension, N/m; C – concentration, %.

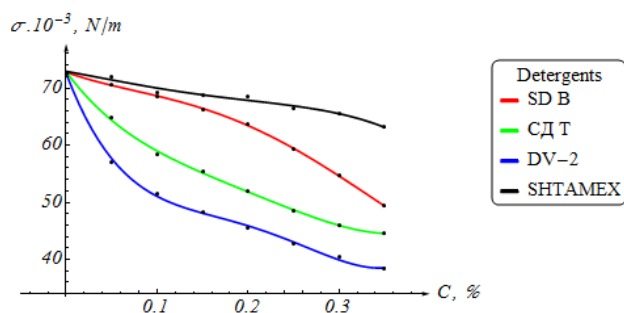


Fig. 2 Dependence of surface tension on detergent concentration in deactivating solutions.

The results, received after graphic differentiation of dependences Fig.2, give the amounts of surface activity, shown in Table2.

Table 2. Surface activity of detergent solutions

detergent t, °C	DV-2	SD „T“	SD „B“
10°C	-81,0171	-64,8325	-50,494
20°C	-82,5559	-64,8457	-56,38
30°C	-82,6505	-65,8962	-60,4664
40°C	-83,8558	-66,8449	-66,6501

Experiments have been conducted in temperature interval from 10°C to 40°C, which is the most suitable for eliminating consequences caused by radioactive contamination. Figure 3 shows the correlation between surface activity and the temperature of synthetic detergents SD„T“, SD„B“ compared to DV-2.

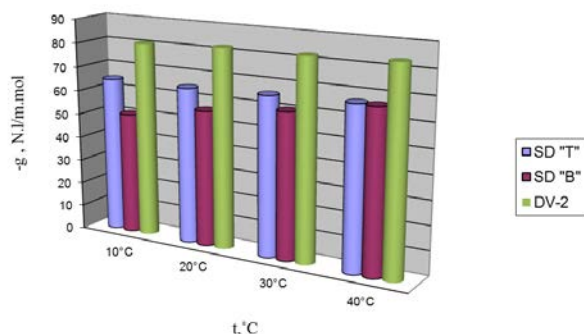


Fig. 3 Dependence of surface activity on temperature of different synthetic detergent solutions.

It is clear from table 2 and fig.3, that the surface activity is lower than that of DV-2, which means that their concentration in deactivating solutions is to be increased in relation to that of DV-2. When temperature is 40°C it does not influence the detergents significantly.

It is obvious from the histogram fig.3, that surface activity of DV-2 has the highest absolute value in comparison to synthetic detergents, object of the research. SD „T“ is adsorbed on the surface 18,9% less than DV-2 at 20°C surface activity of SD „B“ is 45 % lower than that of DV-2.

4. Conclusion:

1. With the usage of graphic differentiation of correlation between concentration and surface tension and the help of applied software product numerical values of deactivating

solutions surface activity have been received which also serve as a base for quantitative and qualitative evaluation of their wettability.

2. It has been determined that water solutions of detergents based on sodium salt of alkyl derivatives (with 10-16 carbon atoms) of benzene sulphotoacid with concentration 0,2 % ÷ 0,35 %. Are applicable for deactivation.
3. The above stated empiric correlations of surface tension and concentration can be applied after statistic processing of experimental results.

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CALCULATING TECHNICAL SCATTERING FULL ERROR FOR EJECTION RELEASE BOMB

ИЗЧИСЛЯВАНЕ НА ПЪЛНАТА ГРЕШКА НА ТЕХНИЧЕСКОТО РАЗСЕЙВАНЕ ПРИ ПРИНУДИТЕЛНО ПУСКАНЕ НА БОМБАТА

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Abstract: The error of aviation bombs mission use is sum of aiming error and technical scattering error. Technical scattering full error is sum of partial errors. Technical scattering full error of aviation bomb for ejection release is determined.

Keywords: technical scattering full error, bomb

1. Introduction

The expression of the error of aviation bombs mission use ξ can be written in the following way:

$$(1) \quad \xi = \xi_a + \xi_t,$$

where ξ_a is the error in solving the aiming problem;

- ξ_t error caused by bombs technical scattering.

Diversions at the initial conditions of bombs movement are the main reason for technical scattering of the bomb explosion points [3]. Another important reason for technical scattering is diversion of ballistic bomb qualities from nominal ones.

Technical scattering caused by the setting is along the course of flight (in the longitudinal plane).

Technical scattering full error of the i bomb $\Delta\xi_{ti}$ is presented as a sum of errors with partial reasons [1]:

$$(2) \quad \Delta\xi_{ti} = \sum_{j=1}^n \Delta\xi_{tij},$$

where j is a symbol of partial reason;

n – the number of reasons.

Each partial error $\Delta\xi_{tij}$ is divided into a group error, equal for all bombs and expressed in shifting the whole bombs series and individual – displacing the length of the series and redistributing the bombs in the series.

Considerable partial errors are:

- $\Delta\xi_{ti}$, error of delay and “disorder” of the moment of dropping, caused by the errors of control system discharge and the errors in the time of moving at the initial section;

- $\Delta\xi_{t0}$, error of oscillation of bomb path, caused by diversion of bomb axis from the tangent in the process of discharge and causing angular velocity of the bomb;

- $\Delta\xi_{tm}$, error, caused by different levels between points of dropping and compartment (inner suspension);

- $\Delta\xi_{tv}$, error caused by the aircraft rate in value and direction in the process of successive bomb dropping and the change in bomb velocity at the initial part of moving.

The full technical scattering error caused by the discharge process is a sum of the partial errors.

$$(3) \quad \Delta\xi_{ti} = \sum_{j=1}^n \Delta\xi_{tij} = W_{\xi} \Delta t_i + \frac{\partial A}{\partial C_{x0}} \Delta C_{x0} + \frac{\partial A}{\partial V} \Delta V_i + \frac{\partial A}{\partial \lambda} \Delta \lambda_i,$$

where

$$\Delta V_i = \Delta V_i^{(1)} + \Delta V_i^{(2)};$$

$$\Delta \lambda_i = \Delta \lambda_i^{(1)} + \Delta \lambda_i^{(2)}.$$

2. Results and Discussion

The odd movement of each bomb at the initial part can be considered as a diversion of real values of initial parameters from predicted values.

Differences in corresponding values $x_b - x_b^r, y_b - y_b^r, \dots$ and so on for the moment of time t_d are diversion of real movement parameters from predicted at the surrounding aircraft area. They are caused by bomb disturbances. Outside disturbance zone and when there is a full bomb oscillation damping, real movement will be distinguished by predicted one only by difference in movement parameters at the surrounding aircraft area. That is why movement parameters at the surrounding aircraft area are considered as initial movement conditions.

Using the formula (3) we have technical scattering full error assessment for fighter bomber at horizontal flight with following data [2]:

- airplane mass - $m=15480$ kg;
- airplane weight - $G=mg=1.5186 \cdot 10^5$ N;
- wing area - $S=34.5$ m²;
- airplane rate - $V=250$ m/s;
- flight altitude - $H=1000$ m.

The study is for practical aviation bomb P-50-75.

When there is bomb ejection release equations for mass center movement are [1]:

$$(4) \quad \begin{aligned} \bar{x} &= \left[\frac{1}{2} (n_{bx} - n_x) g + \omega_z v_y \right] t^2 + \frac{1}{3} \omega_z (n_{by} - n_y) g t^3; \\ \bar{y} &= v_y t + \frac{1}{2} (n_{by} - n_y) g t^2 - \frac{1}{6} \left[2 \omega_z g (n_{bx} - n_x) + \omega_z^2 v_y \right] t^3. \end{aligned}$$

Having in mind that [1] $x_b = x_a + \bar{x} + x_0$, $y_b = y_a + \bar{y} + y_0$, where $x_0 = y_0 = 0$, $x_a = Vt$, $y_a = 0$ and using formula (4) we receive real parameters for bomb movement.

$$\begin{aligned}
\bar{x}_b &= Vt_y + \left[\frac{1}{2}(n_{bx} - n_x)g + \omega_z v_y \right] t_y^2 + \frac{1}{3}\omega_z(n_{by} - n_y)gt_y^3; \\
\bar{y}_b &= v_y t_y + \frac{1}{2}(n_{by} - n_y)gt_y^2 - \frac{1}{6}[2\omega_z g(n_{bx} - n_x) + \omega_z^2 v_y] t_y^3; \\
\dot{\bar{x}}_b &= V + 2 \left[\frac{1}{2}(n_{bx} - n_x)g + \omega_z v_y \right] t_y + \omega_z(n_{by} - n_y)gt_y^2; \\
\dot{\bar{y}}_b &= v_y + (n_{by} - n_y)gt_y - \frac{1}{2}[2\omega_z g(n_{bx} - n_x) + \omega_z^2 v_y] t_y^2.
\end{aligned}$$

Predicted coordinates parameters for bomb movement:

$$\begin{aligned}
x_b^r &= Vt_y; \\
y_b^r &= -\frac{gt_y^2}{2} - v_y t_y; \\
\dot{x}_b^r &= V; \\
\dot{y}_b^r &= -gt_y - v_y.
\end{aligned}$$

- real coordinates

$$\begin{aligned}
\bar{x}_b &= 250t_y - 4.55t_y^2 + 0.011t_y^3; \\
\bar{y}_b &= -5t_y - 3.537t_y^2 - 0.014t_y^3; \\
\dot{\bar{x}}_b &= 250 - 9.103t_y + 0.033gt_y^2; \\
\dot{\bar{y}}_b &= -5 - 7.074t_y - 0.043t_y^2.
\end{aligned}$$

- predicted coordinates

$$\begin{aligned}
x_b^r &= 250t_y; \\
y_b^r &= -4.905t_y^2 - 5t_y; \\
\dot{x}_b^r &= 250; \\
\dot{y}_b^r &= -9.81t_y - 5.
\end{aligned}$$

In the border of disturbance zone for coordinate $y = y_{bd} = -1.5$ m we define t_y :

- real movement

$$t_y = 0.254 \text{ s}.$$

- predicted movement

$$t_y^r = 0.242 \text{ s}.$$

The difference between real and predicted bomb movement in the disturbance zone is assessed by formulas:

$$\begin{aligned}
\Delta t_d &= 0.012 \text{ s}; \\
\Delta x_b &= 2.679 \text{ m}; \\
\Delta \dot{x}_b &= -2.312 \text{ m/s}; \\
\Delta \dot{y}_b &= 0.576 \text{ m/s};
\end{aligned}$$

Technical scattering full error is assessed by formula (3) and airplane ground velocity W_ξ is assessed by formula:

$$(7) \quad W_\xi = V + U,$$

where U is the wind velocity. We assume that $U = 10$ m/s. Then airplane ground velocity is $W_\xi = 260$ m/s.

Partial error $\Delta \xi_{tw}$:

$$\Delta \xi_{tw} = W_\xi \Delta t_d = 3.12 \text{ m}.$$

Resistance coefficient increasing ΔC_{xb} is received by formula:

$$\Delta C_{xb} = 1\% C_{xb} = 0.6146 \cdot \frac{1}{100} = 0.00614.$$

After solving the ballistic problem we receive the partial error, caused by ΔC_{xb} :

$$\Delta \xi_{tCxb} = \frac{\partial A}{\partial C_{xb}} \Delta C_{xb} = 4 \text{ m}.$$

Errors $\Delta V^{(2)}$ and $\Delta \lambda^{(2)}$, caused by bomb movement in the disturbance zone are received by formulas:

$$\Delta V^{(2)} = \Delta \dot{x}_b = -2.312 \text{ m/s};$$

$$\Delta \lambda^{(2)} \approx \frac{\Delta \dot{y}_b}{\dot{x}_b} = 0.13^\circ.$$

Partial error is calculated by formula:

$$\Delta \xi_{tw} = \frac{\partial A}{\partial V} \Delta V^{(2)} + \frac{\partial A}{\partial \lambda} \Delta \lambda^{(2)} = -6.3 + 6.3 = 0 \text{ m}.$$

Technical scattering full error is calculated by formula:

$$\begin{aligned}
\Delta \xi_{ij} &= \sum_{j=1}^4 \Delta \xi_{ij} = W_\xi \Delta t_d + \frac{\partial A}{\partial C_{xb}} \Delta C_{xb} + \frac{\partial A}{\partial V} \Delta V^{(2)} + \frac{\partial A}{\partial \lambda} \Delta \lambda^{(2)} = \\
&= 3.12 - 4 - 6.3 + 6.3 = -0.88 \text{ m}.
\end{aligned}$$

3. Conclusions

From so done calculations for technical scattering full error for ejection release bomb we see that partial errors $W_\xi \Delta t_d$, $\frac{\partial A}{\partial \lambda} \Delta \lambda^{(2)}$ have positive sign. Partial errors $-\frac{\partial A}{\partial C_{xb}} \Delta C_{xb}$, $\frac{\partial A}{\partial V} \Delta V^{(2)}$ have negative sign. As a result that full error decreases.

Technical scattering full error for ejection release bomb is significantly less than an absolute value of the same free release bomb.

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CLOUD TECHNOLOGIES AND MODERN SOFTWARE SOLUTIONS FOR MANAGING AND REWARDING OF STAFF

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Abstract:

Human resource management is an important element of the strategy and policy of any organization. Application of systems for automated execution of activities related to the management and remuneration of human resources gives competitive advantages of organizations. The article identified the main systems and forms of software applications for managing human resources in Bulgaria and analysis of their essential functions. Presented are the features and benefits of cloud technologies in process automation in human resources management and the risks and disadvantages inherent in their use. The recommendations on the use of cloud technologies and software solutions for managing and rewarding of staff in the organization.

KEYWORDS: CLOUD TECHNOLOGIES, SOFTWARE REWARDING, INFORMATION TECHNOLOGY, PERSONNEL, WAGE, CONTEMPORARY FORMS

1. Introduction

Nowadays managers of organizations realize the need to take adequate, accurate and timely solution for the management of human resources. Decision making related to staff is impossible without full information support of processes and information processing with modern automated systems. Consolidation of information activities related to human resources management with information on the overall activities of the organization provides a link between them and facilitates the management of business processes.

The application of software for human resource management supports activities related to the recruitment and selection of staff, effective organization of labor, tracking key indicators of performance and efficiency. Almost every organization in Bulgaria uses software for managing human resources [1].

Most of them develop more 20 years and are updated more often than any other type of software.

The development and renovation of business-oriented software is implemented in the following areas:

- needs and requirements of users;
- development of information technology;
- Changes in regulations related to the tax and labor laws in the country.

1. IT business applications

Development of IT business applications and service activities related to human resources management passes in three phases:

- Automation of payroll calculation;
- Automation of accountability related to staff in the organization;
- Automation of the processes of decision-making related to human resources management.

Initially computer processing includes routine and most labor-intensive operations related to the calculation of wages, accruals and deductions for social security and health insurance and taxes.

These operations are suitable for automation, as they are computing, clearly regulated and can easily fit into the algorithms [1].

At a later stage to the functionality of the software added new opportunities for gathering and storing information:

- the composition and structure of the staff in the organization, systematized in units and departments;
- Files for accounting personnel data for each employee, the history of their changes and others similar functions [1].

Automation of processes in making decisions related to human resources management is related to coverage of the parameters that would be difficult formulated. If the software application must support profile for the competence of the

employee, and in it than the traditional staffing accountability information (education, employment, etc.), account and not subject to precise measurement indicators such as the ability to adapt, leadership skills, ability to work in a team, etc. [1, 2].

There are Five Key Functions of an HRMS System [3]:

- Payroll
- Benefits Administration
- Training Systems
- Recruiting
- HR Metrics

According to analysts at Forrester Research [1] "modern Forrester Research blocks unevenly distributed across three levels: "User", "Strategic" and "Field", which include:

Self - service interaction layer:

- Employee self-service;
- Manager self-service;
- Employee communications;
- Management reporting and analysis.

Learning management processes:

- Training administration;
- Learning content management;
- Learning delivery;
- Recruitment processes;
- Candidate sourcing.

Workforce management processes:

- Time and attendance;
- Forecasting and scheduling;
- Absence management;
- Employee records and personnel actions;
- Benefits administration;
- Payroll;
- Position management;
- HR compliance.

Software companies are in a new stage of development in terms of the software available on the market. The development of automated systems for wage becomes more complicated for firms developing such products process as legislation in the country continuously compounded. The changes came into force on 01.01.2014 г. (Declaration 1 is equal to the Declaration 6 and simultaneous submission) difficult as companies working with software applications for salary and companies that develop them [2].

Decisions on staff remuneration reflects the strategy and policy of the organization in the field of human resources and the result of evaluation of performance of staff. Highlights of remuneration are:

- financial reward (monetary, cash);
- non-financial remuneration (non-monetary, moral).

Characterization of wages in terms of national legislation and international labor law proves that pay is an important material incentive to work.

Classic element of the remuneration of labor of employees is wages as consideration of the work on labor contract. Wages monetary remuneration determined in accordance with the agreement under a contract for hire, the employer shall pay employees for their service.

Salary is a structure element of the cost of labor. In parallel, it is also independent economic category, which is determined by factors outside the market. Wage focus socio-economic, political, and legal and other processes in society.

Complete and accurate classification systems and varieties of salary is a complex task, as is practice they are considered trade secret and information about them is not disclosed [4, 5]. In practical activities most commonly used systems of wages are:

- Payment of the length of the work - the amount of the salary is determined by multiplying the amount of waste during working days or hours daily and hourly rate for a particular job or position;

- Payment according to the output - an assessment criterion for the work they have made workers by the amount of output;

- Percentage fee - in its use as a criterion for evaluation of the work using the amount of revenue realized a worker as an employee or group of workers;

- Combined payment - criteria are output as output and hours worked.

In organizations apply other forms of wages such as: pay according to work efficiency, merit, etc.

Notwithstanding the application system or form of wages, it should be competitive (respecting market levels of remuneration), deservedly (according to the quantity and quality of the work), and to take into account the influence of factors affecting it [6, 7].

Almost all companies use software to calculate the wages according to their needs. SMBs are satisfied with basic opportunities for formation and calculation of remuneration and insurance and tax rates. Automation of management of human resources of larger companies with distinct divisions requires a richer functionality - maintaining a database of job applicants modules for training and qualification of personnel options to compile specific information and analyzes, etc.

- Core HR encompasses the three traditional human resources management functions:
- benefits administration - time off, medical/dental/life insurance policies;
- personnel tracking - Centralizes employee data such as contact information, past employment and demographic information;
- payroll – tracking employee salaries, bonuses, health and other deductions; calculates withholding for taxes.

The companies will require these functions when they have reached a critical mass of employees e.g. when, for instance, manually running payroll and managing employees with spreadsheets becomes difficultly a task.

Workforce management comprises of software solutions intended to effectively track workforce. These solutions are for organizations whose employees work in shifts, and include applications to track time and attendance, monitor compliance with labor laws and usually include payroll functionality.

Strategic HR involves growing the company by attracting and developing the best people and provide a combination of applicant tracking and recruiting, learning management as well as performance review functionality. This type of software ensure that a company is using its staff as efficiently as possible, and that employees are continuing to grow and develop, increasing employee satisfaction and retention rates.

- Workforce Management
 - Time and attendance - Helps staff track employee attendance and absences. Many software solutions track accrual and usage of sick days. Rules-based engines provide

alerts when employees miss or perform established amounts of work.

- Provides functionality for scheduling employee shifts and attendance to ensure compliance with staffing needs. Systems can schedule employees across departments, locations and projects, and provide alerts to employees when schedules change and when staffing levels are inadequate.

- Strategic HR

- Applicant tracking systems - Provides a centralized database that lets recruiters store applicant information and employment applications throughout the application process. Features include candidate tracking, applicant status monitoring and direct integration with other HR applications.

- Employee evaluation - Also known as performance review software, these applications offer a centralized system where supervisors can conduct and track reviews with employees. Features performance measuring, tracking and management by objectives.

- Learning and development - Established a centralized hub to monitor new employee training and the ongoing skills development of existing employees. Features include content authoring and management, curriculum and certification path definition.

2. Automated salary

Companies developing software for wage offer different versions of software applications with the functionality and parameters suitable for large and small companies, to companies with different numbers of staff with different financial capabilities and different activity. In our country have created a large number of software systems for human resources, which include a wide range of features that can be summarized in the following areas:

Omex 2000 [8] is an integrated software system that is designed for automation of departmental activities "Wages" and "Personnel" in all types of companies, regardless of the form of ownership and the system of remuneration. The program is built on modern tools and technology and is consistent both with the frequent changes in employment, tax and social legislation and with the rapid development of information technology. The system works with a single database, which frees the user to use parts of it without compromising the integrity of the information.

The rich functionality of the system, timely and professional support make the software Omex 2000 reliable and preferred means of supporting the management and remuneration of human resources in organizations.

TERES [9] is a system which automates the work of planning and reporting of labor, wage and fee statements in civil contracts. Liaise via file export to the most common accounting products with different types of banking software and a personal register of the National Social Security Institute.

Microinvest "Work, salary and personnel" Pro [10] is a comprehensive system for processing and control of data for company staff. The program offers features such as access control, entering and editing data from remote workstations. Has a complete set of forms and documents necessary for organization of the activity of bringing staff; preparation of data files for export to the National Revenue Agency and the National Social Security Institute; generating intensive inquiries as Certificates of retirement, references to statistics, etc..

Program suitable for companies with different activity is Payroll Atlas [11]. The system is a software solution for the department "Labor and wages", intended for the implementation of personnel policy and management wages. The program provides estimates of wages with opportunities to use monthly, daily and hourly tariff rates and individual earnings, calculating regulated by law charges and deductions, etc.

SysHR [12] is a system for automated calculation of accruals, deductions and remuneration of staff to meet the regulatory requirements in the country. The system maintains information on wages and personal files of the employees of the

company. Used by financial institutions, manufacturing companies, hotels, trading companies and budget organizations. Advantage of the system SysHR new type of service - SysHR for Rent.

The new service SysHR for Rent provides its customers to use the same product for rent, it saves significant investment, work pressure and excessive, unnatural responsibility for the preservation and maintenance of the database.

The initial cost of license fees, software, equipment, certainly borne by the organization, providing software.

With the new type of service SysHR For Rent consumer guarantee:

- modern technology platform - Oracle;
- full functionality of the system "Management of human resources and salary";
- maximum flexibility of service according to user needs;
- high level of security for the database, guaranteed by highly qualified specialists and modern equipment;
- modern means to protect information from unauthorized access over the Internet - electronic certificates and encrypted connections;
- continuous process of work – 24 x 7;
- rapid response and recovery capability of the system in crisis;
- data protection technical failures, disasters, accidents, theft of office equipment, etc.;
- reflecting the normative changes in the system SysHR For Rent;

-ensuring and improving accountability to the National Insurance Institute.

According Common Features HR Software can be summarized as [13]:

3. Cloud HR software and Payroll calculation

-Automated payroll calculation than speed, timeliness and ease of use allows for the use of information from past periods, automated software updates, which in the dynamic change of law is essential.

-Manual payroll calculation is applied less frequently. Preferably of companies with a small number of staff (one,two), as in these cases it is advisable to invest in the purchase of software.

-Autoskrining – functions of processing and calculation of salary transferred to specialized companies in these activities (accountants, etc.). It is preferred by small companies [14].

The companies start a new war for talent, this \$14+ billion market continues is with growth - 57 % of companies plan to make a major new HR software purchase in the next 18 months.

According J. Bersin there are the top 7 reasons of growth of HR software:

1. HR software systems are aging.

The average HRMS system in large companies today is more than 5 years old.

2. Cloud HR software is now easy to buy.

Nearly every major HR software provider now offers their solution in the cloud, making it possible for corporate HR managers to stop of upgrading systems every year. And once the company buy a cloud-based system, it is out of the cycle of major upgrades every few years because the vendor does this.

3. New User Interfaces are a top driver for replacement.

Our research now shows that the driver of change is the need for a more compelling, consumer-like, experience. Most of the vendor solutions now have mobile applications also, enabling employees to manage their vacation, time sheets, and employee directories on the road.

4. Companies have too many systems and are ready to consolidate.

Only 13% of organizations have a single HR system and on average companies have 3-4 different HR applications (one for learning, another for recruiting, for example).

5. The Potential for Big Data Analytics

Second on the list of buying criteria is the desire to create better talent analytics. While much of the core HR technology has now become a commodity, analytics is still a new area of technology and vendor solutions here vary greatly.

6. Cloud Technology makes it Easier to Switch Vendors.

Since more and more companies now have cloud-based systems for recruiting, learning, and other HR applications, it is now easier than ever to switch. Unlike traditional software which is highly customized by IT, these new systems can be replaced.

7. Talent become one of the most important issues for CEO of the company

For the global economy recovers more and more companies realize that human resource are their biggest challenge. Strategic recruiting, employee development, social networking, and internal employee communications are all critical business issues. The hottest categories according J. Bersin are:

- New generation of recruiting (social recruiting tools, assessment, Big Data)
- Mobile applications (mobile learning, recruiting, collaboration, and employee management)
- Analytics (Big Data tools to analyze the job market, recruitment advertising), and new tools to enable social learning, knowledge management, and training administration.

It's a great time to „be buying and selling HR software today: lots of options and they are all getting better“.

CONCLUSION

Notwithstanding the application system and form of remuneration in the organization and management decision taken for the implementation of an automated system to calculate the wage is necessary to take into account the following objectives:

- attracting and retaining highly qualified and experienced staff;
- maintaining high motivation by providing remuneration commensurate with performance,
- improving the image and competitiveness of the organization;
- maintaining high performance and quality of the products and services to be achieved as the objectives of the organization and the personnel working in it.

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